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Standard X-ray Diffraction Powder Patterns



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Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, Marlene Cook Morris,
Eloise H. Evans, and Linda Ulmer



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Errata

Circular 539

Vol. 1, Page 50, In the pattern of Swanson and Tatge, the d -values 0.8576, 0.8557, 0.8467, 0.8412, and 0.8383 should have the following hkl values, 422, 511, $\bar{5}13$, 333, and 206.

Vol. 2, Page 46, Lattice constants paragraph, column 1, line 3: Puma should read Pnma. This change was made in the Vol. 2 reprint.

Vol. 3, Page 54, On the line below hkl 121 insert hkl 012; on the line below hkl 200 insert hkl 031; hkl 040 should read 211; delete hkl values 230 and 410 and all those following 421.

Vol. 5, Page 10, Column 1, bottom line, the index of refraction should read 1.710. Page 11, In pattern of Swanson, Gilfrich, and Ugrinic, for hkl 721 d should read 2.078.

Page 43, Reference No. 3: The fourth author's name should be F. E. Sennett.

Vol. 8, Page 42, Column 1: The density should be 4.697.

Page 65, Ti_5Si_3 should have 2 molecules per unit cell and the density 4.376.

Vol. 9, Page 6, $(\text{NH}_4)_2\text{PtBr}_6$ table: Cu radiation applies to entire table.

Errata—Continued

Page 19, *hkl* 102 should be 012.

Page 47, The density of K_3ZrF_7 should be 3.123.

Monograph 25

Sec. 1, Page 10, Lattice constants table: headings *a b c* should read *b c a*.

Page 12, The title should read: Erbium Gallium Oxide 3:5. . . .

Sec. 2, Page 1, Column 2 line 11: potassium nitroso chlororhenate should be potassium nitroso chlororuthenate.

Page 2, In the left hand column, the sentence beginning in the seventh line from the bottom should read: Factors for converting integrated intensities to peak height intensities are on the left side of the chart.

Page 8, $CdWO_4$ space group should be C_{2h}^4 —P2/c (No. 13).

Page 11, Spectrographic analysis should read: 0.01 to 0.1 percent sodium and

Page 34, The intensity of the line at $d=4.21$ should be 61. Insert the reading: $hkl=102$, $d=3.94$, $I=2$.

Page 35, Reference No. 7 should read: Helen M. Ondik, to be published in *Acta Cryst.*

Addenda

Monograph 25

Sec. 2, Page 22, Insert this data:

<i>hkl</i>	<i>d</i>	<i>I</i>	<i>a</i>
930	1.2843	<1	12.184
965	1.0225	<1	12.184
10.8.2	.9398	<1	12.181
13.5.0	.8408	<1	12.184
14.3.3	.8329	<1	12.184

Sec. 2, Page 35, Add this data: The sample is optically negative and the indices of refraction are $N_\alpha=1.440$, $N_\beta=1.458$, $N_\gamma=1.474$, and $2V \cong 90^\circ$.

Standard X-ray Diffraction Powder Patterns

The eleven previous volumes in this series are available from the Superintendent of Documents, U.S. Government Printing Office, Washington 25, D.C., as follows:

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 3—Data for 51 Substances

Howard E. Swanson, Marlene Cook Morris,¹

Eloise H. Evans,¹ and Linda Ulmer

Standard x-ray diffraction powder patterns are presented for the following fifty-one substances: $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$, (mullite); $(\text{NH}_4)_2\text{BeF}_4$; NH_4BF_4 ; Sb_2Se_3^* ; Sb_2Te_3^* ; As_2O_3^* , claudetite; $\text{BaBr}_2 \cdot \text{H}_2\text{O}^*$; BaSnO_3 ; BiPO_4 (monoclinic); BiPO_4^* (trigonal); BiVO_4^* (tetragonal); BiVO_4^* (monoclinic); Bi_2Te_3 , (tellurobismuthite); Bi_2O_3 , (bismite); $\text{Cd}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}^*$; CdSO_4 ; CdTe ; $\text{Ca}_5\text{F}(\text{PO}_4)_3$, (fluorapatite); CeNbTiO_6^* , (eschynite); $\text{Cs}_2\text{CrO}_4^*$; CsF ; $\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}^*$; $\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}^*$; CuSO_4 , (chalcocyanite); DyAsO_4^* ; ErAsO_4^* ; EuAsO_4^* ; GaAs^* ; HoAsO_4^* ; InAs ; LaAsO_4^* ; LaNbTiO_6^* ; Li_3PO_4 , (lithiophosphate) low form; Li_3PO_4 high form; $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$, (struvite); KClO_3 ; KLiSO_4^* ; K_3CrO_8^* ; $\text{K}_2\text{Zn}_2\text{V}_{10}\text{O}_{28} \cdot 16\text{H}_2\text{O}^*$; $\text{Rb}_2\text{CrO}_4^*$; AgSbTe_2^* ; $\text{NaMg}_3\text{Al}_3\text{B}_3\text{Si}_6\text{O}_{27}(\text{OH})_4^*$, dravite; $\text{Na}_3\text{P}_3\text{O}_9$; $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$; SnF_2^* ; $\text{SrO} \cdot \text{B}_2\text{O}_3^*$; TbAsO_4^* ; TlCrO_4^* ; TmAsO_4^* ; TiO_2 , brookite; and ZnTe . Twenty-one are to replace patterns already given in the X-ray Powder Data File issued by the American Society for Testing and Materials, and thirty patterns indicated by asterisks are for substances not previously included. The patterns were made with a Geiger counter x-ray diffractometer, using samples of high purity. When possible, the d -values were assigned Miller indices determined by comparison with calculated interplanar spacings and from space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

INTRODUCTION

The X-ray Powder Data File [1]² is a compilation of diffraction patterns from many sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. The National Bureau of Standards in its program³ for the revision and evaluation of published x-ray data for the X-ray Powder Data File presents data in this report for 51 compounds. This compilation is the thirteenth of a series of "Standard X-ray Diffraction Patterns."⁴ The designation "Circular 539" used for the first 10 volumes has been discontinued in favor of the new series, "Monograph 25." This compilation is the third section of the new series Monograph 25. Included are patterns recommended to replace data on 26 cards now present in the File. The other patterns are for 30 compounds not included in the File. These compounds are: antimony selenide; antimony telluride; arsenic oxide, claudetite; barium bromide monohydrate; bismuth orthophosphate (trigonal); bismuth orthovanadate (tetragonal); bismuth orthovanadate (monoclinic); cadmium perchlorate hexahydrate; cerium niobium titanium oxide, eschynite; cesium chromate; cobalt fluosilicate

hexahydrate; cobalt perchlorate hexahydrate; dysprosium arsenate; erbium arsenate; europium arsenate; gallium arsenide; holmium arsenate; lanthanum arsenate; lanthanum niobium titanium oxide; potassium lithium sulfate; potassium perchromate; potassium zinc decavanadate 16-hydrate; rubidium chromate; silver antimony telluride; sodium magnesium aluminum boron hydroxy silicate, dravite; stannous fluoride; strontium 1:1 borate; terbium arsenate; thallium chromate; and thulium arsenate.

The experimental procedure and general plan of this Monograph section 3 have not changed greatly from previous publications. However, the basic technique is discussed, in this section, with minor changes.

Powder data cards. Under this heading are given the Powder Data File card numbers, the three strongest lines, and the literature references for each card. Cards listed through the 1962 index to the Powder Data File are included in the table.

Additional published patterns. Literature references for patterns that have not been published as Powder Data cards are listed.

NBS sample. Many of the samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory by J. deGroot. Unless otherwise noted, the spectrographic analyses were done at NBS after preparation of the sample was completed. The limit of detection for the alkali elements was 0.05 percent for the spectrographic analysis. A microscopic inspection for phase purity was made on the nonopaque materials during the refractive index determination. Another check of phase purity was

¹ Research Associate at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods.

² Figures in brackets indicate the literature references at the end of each section of this paper.

³ This project is sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods. This committee is composed of members from the American Society for Testing and Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

⁴ Other volumes were published as follows: Circular 539 Vol. 1 and Vol. 2, June 1953; Vol. 3, June 1954; Vol. 4, March 1955; Vol. 5, October 1955; Vol. 6, September 1956; Vol. 7, September 1957; Vol. 8, April 1959; Vol. 9, February 1960; Vol. 10, September 1960; Monograph 25 Section 1, March 1962; and Section 2, May 1963.

usually provided by the x-ray pattern itself, when it was indexed by comparison with theoretical d -values. Treating the sample by appropriate annealing, recrystallization, or heating in hydrothermal bombs improved the quality of most of the patterns. The refractive index measurements were made by grain-immersion methods in white light, using oils standardized in sodium light, and covering the range 1.40 to 2.00.

X-ray techniques. At least three patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particle-size smaller than $10\ \mu$. [2]. In order to avoid the orientation effects when samples are packed or pressed, a sample holder was made that had an extended rectangular cavity open at its top face and end. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall. (See fig. 1.) The powdered sample was then drifted into the remaining end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample surface could be exposed to the x-ray beam (as shown in fig. 2). To powders that did not flow readily or were prone to orient excessively, approximately 50-volume percent of finely-ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line. Additional patterns were obtained for d -value measurements. Specimens for these patterns were prepared by packing into a shallow holder a sample containing approximately 5-wt percent tungsten powder that served as an internal standard. When tungsten lines were found to

interfere, 25 percent silver was used in place of tungsten. If the internal standard correction varied along the length of the pattern, linear interpolations were used for the regions between the peaks of the standard. For low values of 2θ , the pattern peak was measured in the center, at a place averaging about 75 percent of the peak height. For higher values of 2θ , where the α_1 and α_2 peaks were separated, the α_1 peak was measured in the same way. The internal standard correction appropriate to each region was then applied to the measurement of 2θ . The internal standard lattice constants used were $3.1648\ \text{\AA}$ for tungsten and $4.0861\ \text{\AA}$ for silver at $25\ ^\circ\text{C}$. as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at $25\ ^\circ\text{C}$, using either filtered copper or cobalt radiation ($K\alpha_1$), having the wavelengths $1.5405\ \text{\AA}$, and $1.7889\ \text{\AA}$, respectively.

Structural data. For cubic materials a value for the lattice constant was calculated for each d -value. However, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the large-angle region of the pattern. The unit cell values for each noncubic substance were determined by means of a least-squares calculation made on the IBM 7090, using those d -values for which only one set of Miller indices could be assigned. The number of significant figures reported for d -values in the NBS pattern is limited by the quality of each sample as indicated by residuals obtained from least squares refinement. A portion of the indexing and cell refinement calculation was performed on a Burroughs B 220 computer at the United States Geological Survey using a program developed by H. T. Evans, Jr.



FIGURE 1



FIGURE 2

D. E. Appleman, and D. Handwerker. Lattice constant errors are given only for data refined on that program and are based on least squares refinement of the variance-covariance matrix derived from the unweighted $\Delta\theta$ residuals.

Published unit cell data in kX units were converted to angstrom units using the factor 1.00202 as recommended by an international conference of crystallographers [4].

The space groups are listed with both the Schönflies and short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography [5].

Orthorhombic cell dimensions are presented according to the Dana convention [6] $b > a > c$.

The densities calculated from the NBS lattice constants are expressed in grams per cubic

centimeter and are computed with atomic weights based on carbon 12 [7], and the Avogadro number (6.02252×10^{23}).

References

[1] Index to the X-ray Powder Data File, American Society for Testing and Materials, 1916 Race Street, Philadelphia 3, Pa. (1962).
[2] L. Alexander, H. P. Klug, and E. Kummer, Statistical factors affecting the intensity of x-rays diffracted by crystalline powders, J. Appl. Phys. **19**, No. 8, 742-753 (1948).
[3] E. R. Jette and F. Foote, Precision determination of lattice constants, J. Chem. Phys. **3**, 605-616 (1935).
[4] The conversion factor for kX units to angstrom units, J. Sci. Inst. **24**, 27 (1947).
[5] International Tables for X-ray Crystallography, **1**, 1952.
[6] Dana's System of Mineralogy, **1**, 6 (1944).
[7] International Union of Pure and Applied Chemistry, Chem. Eng. News, Nov. 20, 43 (1961).

Aluminum 3:2 Silicate (mullite)* $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$ (orthorhombic)

Powder data cards

Card number	Index lines	Source
6-0258	3. 38 2. 20 3. 41	F. H. Gillery [1].
10-394	3. 39 3. 42 2. 54	H. Scholze [2] 1955.

Additional published patterns. Norton [3] 1925, Navias and Davey [4] 1925; Wyckoff, Grieg, and Bowen [5] 1926; Mark and Rosbaud [6] 1926; Nahmias [7] 1933; Comeforo, Fischer, and Bradley [8] 1948; and Kurylenko [9] 1952.

NBS sample. The sample of aluminum 3:2 silicate was prepared at NBS by C. Robbins. Gamma Al_2O_3 and $\text{SiO}_2 \cdot n\text{H}_2\text{O}$ were mechanically mixed in stoichiometric proportions of $3\text{Al}_2\text{O}_3$ to $2\text{SiO}_2 \cdot n\text{H}_2\text{O}$. This mixture was pressed into pellets and fired at 1400 °C and 1500 °C with little reaction, then remixed and fired in an open system at 1700 °C for 24 hr. Reaction was nearly complete. It was crushed, reground in an agate mortar and refired at 1725 °C for 24 hr. Chemical analysis of the finished product showed 61.6 mole percent Al_2O_3 and 38.4 mole percent SiO_2 instead of the beginning percentages of 60 and 40 in the 3:2 mixture. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent iron, and 0.001 to 0.01 percent each of calcium, chromium, magnesium, manganese, nickel, titanium, and zirconium.

The sample was colorless and optically positive with the indices of refraction $N_\alpha=1.637$, $N_\beta=1.641$, and $N_\gamma=1.652$.

The d -values of the three strongest lines are: 3.390, 3.428 and 2.206 Å.

Structural data. Sadanaga, Tokonami, and Takéuchi [10] in 1962 determined that mullite has the space group D_{2h}^2 -Pbam (No. 55). Wyckoff, Grieg, and Bowen [5] in 1926 determined that mullite has $3/4(3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2)$ per unit cell. Several lattice constants have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
		Å	Å	Å
1926	Wyckoff, Grieg, and Bowen [5].	7. 52	7. 68	2. 86
1928	Taylor [11]-----	7. 51	7. 65	2. 88
1933	Nahmias [7]-----	7. 54	7. 67	2. 90
1952	Kurylenko [9]---	7. 580	7. 689	2. 895
1955	Scholze [2]-----	7. 537	7. 671	2. 878
1960	Agrell and Smith [12].	7. 5582	7. 6878	2. 8843
1962	Sadanaga, Tokonami, and Takéuchi [10].	*7. 583	*7. 681	*2. 8854
1963	National Bureau of Standards at 25 °C.	7. 5456 ±. 0004	7. 6898 ±. 0005	2. 8842 ±. 0002

*These values are for $2\text{Al}_2\text{O}_3 \cdot \text{SiO}_2$.

*Some disagreement exists in the literature as to which ratio or ratios of alumina to silica should be considered for mullite (3:2, 2:1, or both). This sample was prepared as 3:2 at the request of P. Schroth of the Arco Steel Corp. to be used as an identification, diffraction standard for mullite in refractory brick.

The density calculated from the NBS lattice constants is 3.170 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C		<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>		<i>d</i>	<i>I</i>
	\AA			\AA	
110	5.39	48	112	1.3932	<2
200	3.774	8	341	1.3494	6
120	3.428	96	440	1.3462	
210	3.390	100	151	1.3356	12
001	2.886	21	122	1.3290	5
			212	1.3266	
220	2.694	40	511	1.3172	4
111	2.542	52	350	1.3120	3
130	2.428	13	530	1.3004	4
310	2.393	<2	060	1.2814	7
021	2.308	3	251	1.2771	13
201	2.292	19	222	1.2714	6
121	2.206	61	521	1.2630	12
230	2.121	23	600	1.2574	<2
320	2.106	7	132	1.2396	6
221	1.969	2	312	1.2349	2
040	1.923	2	441	1.2199	2
400	1.887	8	260	1.2131	<2
140	1.863	<2	232	1.1924	4
311	1.841	10	531	1.1855	3
330	1.7954	<2	402	1.1457	<2
240	1.7125	6	261	1.1190	1
321	1.7001	14	242	1.1032	4
420	1.6940	10	422	1.0981	5
041	1.5999	20	270	1.0548	<2
401	1.5786	11	171	1.0172	4
141	1.5644	2	252	1.0133	4
411	1.5461	2	370, 522	1.0065	8
331	1.5242	37			
150	1.5067	<2			
510	1.4811	<2			
241	1.4731	<2			
421	1.4605	7			
002	1.4421	17			
250	1.4240	3			
520	1.4046	7			

References

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- [2] H. Scholze, Zum Sillimanit-Mullit Problem, Ber. deut. keram. Ges. **32**, 381-5 (1955).
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- [7] M. E. Nahmias, Bauxites et mullites, étudiées au moyen des rayons X. Z. Krist. **85**, 355-69 (1933).
- [8] J. E. Comeforo, R. B. Fischer, and W. F. Bradley, Mullitization of kaolinite, J. Am. Ceram. Soc. **31**, 254-9 (1948).
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Ammonium Fluoberyllate, $(\text{NH}_4)_2\text{BeF}_4$ (orthorhombic)

Powder data cards

Card number	Index lines	Source
3-0885	2. 48 2. 27 4. 31	The Dow Chemical Co.

Additional published patterns. None.

NBS sample. The sample of ammonium fluoberyllate was obtained from K and K Laboratories, Jamaica, Long Island, N.Y. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, calcium, and silicon.

The sample was colorless, and optically negative with $N_\alpha = 1.397$, $N_\beta = 1.401$, and $N_\gamma = 1.403$.

The d -values of the three strongest lines are: 4.275, 2.478, and 4.312 Å.

Structural data. Hultgren [1] in 1934 determined that ammonium fluoberyllate belongs to the space group D_{2h}^{10} -Pnam (No. 62) with $4[(\text{NH}_4)_2\text{BeF}_4]$ per unit cell. The lattice constants of Mukherjee [2] have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
		Å	Å	Å
1934	Hultgren [1]-----	7. 5	10. 2	5. 8
1945	Mukherjee [2]---	7. 51	10. 41	5. 90
1963	National Bureau of Standards at 25 °C.	7. 645 ±. 001	10. 450 ±. 001	5. 929 ±. 001

The density of ammonium fluoberyllate calculated from NBS lattice constants in 1.698 g/cm³ at 25 °C.

hkl	Internal Standard, Tungsten, $a = 3.1648$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
020	5. 229	5
011	5. 157	15
120	4. 312	90
111	4. 275	100
200	3. 821	36
201	3. 212	< 2
220	3. 085	38
031	3. 003	46
002	2. 962	40
131	2. 794	< 2
112	2. 671	23
040	2. 612	48
230	2. 575	15
310	2. 478	96
122	2. 443	69
231	2. 362	15
202	2. 342	< 2
320	2. 289	75
311	2. 284	< 2
132	2. 164	32
321, 222	2. 136	25
330	2. 056	16
241	2. 027	3
051	1. 970	3
013, 331	1. 942	26
400	1. 911	4
410	1. 879	< 2
250	1. 8339	10
401	1. 8192	2
322	1. 8124	< 2
411, 420	1. 7934	2
251	1. 7526	7
341	1. 7552	< 2
033	1. 7193	3
160	1. 6977	4
133	1. 6765	4
350	1. 6168	< 2
402	1. 6070	5
233	1. 5668	< 2
252, 351	1. 5598	2
510	1. 5124	3
323	1. 4963	< 2
004	1. 4821	6

References

- [1] R. Hultgren, Crystal structures of ammonium beryllium fluoride, *Z. Krist. (A)* **88**, 233-237 (1934).
- [2] P. L. Mukherjee, Crystal structures of metallic fluoberyllates, double fluoberyllates and sulphato-fluoberyllates, *Indian J. of Phys.* **18**, 148 (1945).

Ammonium Fluoborate, NH_4BF_4 (orthorhombic)

Powder data cards.

Card number	Index lines	Source
1-0335	4. 50 3. 55 3. 18	Hanawalt, Rinn, and Frevel [2] 1938.

Additional published patterns. None.

NBS sample. The sample of ammonium fluoborate was obtained from K and K Laboratories, Jamaica, Long Island, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of calcium and phosphorus and 0.001 to 0.01 percent each of iron, titanium, and strontium.

The sample was colorless and had extremely low birefringence and indices of refraction.

The d -values of the three strongest lines are: 4.482, 3.542, and 3.186 Å.

Structural data. Hoard and Blair [1] in 1935 determined that ammonium fluoborate has the space group D_{2h}^{16} -Pbnm (No. 62) and $4(\text{NH}_4\text{BF}_4)$ per unit cell. The cell constants of Hoard and Blair have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
		Å	Å	Å
1935	Hoard and Blair [1].	7. 24	9. 08	5. 65
1963	National Bureau of Standards at 26 °C.	7. 272 ±. 001	9. 063 ±. 001	5. 686 ±. 001

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 26 °C		hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 26 °C	
	d	I		d	I
	Å			Å	
110	5. 668	30	312	1. 808	8
020	4. 528	58	410	1. 782	2
101	4. 482	100	150	1. 759	<1
120	3. 844	51	023	1. 749	<1
200	3. 635	51	142	1. 721	5
021	3. 542	85	322	1. 708	2
210	3. 376	11	411, 123	1. 701	<1
121	3. 186	85	151	1. 680	3
211	2. 902	61	213	1. 653	19
002, 220	2. 839	35	250	1. 622	4
130	2. 792	4	242	1. 593	<1
112	2. 541	45	223	1. 575	3
131	2. 505	12	430	1. 558	2
022	2. 409	12	402	1. 532	1
310	2. 341	23	060, 412	1. 510	<1
230	2. 324	37	303	1. 4933	2
122	2. 286	35	233	1. 4691	<1
040	2. 266	10	043	1. 4535	5
202	2. 238	18	510	1. 4365	4
301	2. 232		161	1. 4316	4
212	2. 176	45	004	1. 4217	2
311, 140	2. 165		260	1. 3954	<1
231	2. 151		520	1. 3848	<1
320	2. 138		441	1. 3755	<1
041	2. 104	11	432	1. 3656	2
141	2. 022	3	521	1. 3459	<1
222	2. 008	3	333	1. 3381	1
330	1. 891	2	062	1. 3344	<1
103	1. 834	2	530	1. 3104	<1
241	1. 821	6	413	1. 2983	2

Ammonium Fluoborate, NH_4BF_4 (orthorhombic)—Continued

The density of ammonium fluoborate calculated from the NBS lattice constants is 1.858 g/cm^3 at 26°C .

References

- [1] J. L. Hoard and V. Blair, The crystal structures of rubidium and ammonium fluoborates, *J. Am. Chem. Soc.* **57**, 1985–88 (1935).
- [2] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, *Ind. Eng. Chem. Anal. Ed.* **10**, 457–512 (1938).

Antimony Selenide, Sb_2Se_3 (orthorhombic)

Powder data cards. None.

Additional published patterns. Dönges [1] 1950.

NBS sample. The sample of antimony selenide was obtained from Semitronics, Inc., Winchester, Mass. It was heated in an evacuated tube at 450°C overnight to obtain a sharper pattern. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent tellurium and

0.001 to 0.01 percent each of aluminum and silicon.

The sample was a dark gray opaque powder.

The d -values of the three strongest lines are: 2.868, 3.162, and 3.253 \AA .

Structural data. Dönges [1] in 1950 determined that antimony selenide has the antimony sulfide structure, the space group D_{2h}^{16} -Pbnm (No. 62), and $4(\text{Sb}_2\text{Se}_3)$ per unit cell.

Lattice constants

		a	b	c
		\AA	\AA	\AA
1950	Dönges [1]-----	11.58	11.68	3.98
1963	National Bureau of Standards at 25°C -----	11.633	11.780	3.985

hkl	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	d	I
	\AA	
110	8.28	7
020	5.89	24
200	5.82	5
120	5.25	55
220	4.14	10
101	3.76	11
130	3.720	32
310	3.682	15
021	3.297	11
231	3.253	71
211	3.162	73
040	2.945	2
400	2.910	4
221	2.868	100
301	2.776	62
330	2.759	10
311	2.703	22
240	2.629	61
420	2.608	22
321	2.513	31
041	2.367	23
340	2.345	13
430	2.337	13
141	2.319	35
411	2.303	12
510	2.282	8
331	2.268	7
250	2.184	35
520	2.164	19
440	2.070	9
431	2.015	35
501	2.010	31
530	2.002	31
151	1.998	23
002	1.989	26
060	1.963	7

hkl	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	d	I
	\AA	
112	1.938	7
160	1.936	7
610	1.913	7
212	1.861	8
620	1.841	3
441	1.837	4
540	1.826	3
351	1.797	8
531	1.788	15
061	1.761	47
312	1.752	20
322	1.698	13
621	1.672	5
710	1.646	5
142	1.632	<1
412	1.628	<1
640	1.619	6
270	1.617	8
720	1.600	12
242	1.586	17
422	1.582	10
370	1.544	8
171	1.568	5

Antimony Selenide, Sb_2Se_3 (orthorhombic)—Continued

Reference

The density of antimony selenide calculated from NBS lattice constants is 5.843 g/cm^3 at 25°C .

- [1] E. Dönges, Über Selenohalogenide des dreiwertigen Antimons und Wismuts und über Antimon (III)-selenid, Z. anorg. Chem. **263**, 280–291 (1950).

Antimony Telluride, Sb_2Te_3 (trigonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of antimony telluride was obtained from Semitronics, Inc., Winchester, Mass. It was heated at 450°C overnight in an evacuated tube to sharpen the pattern. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum and silicon.

The sample was dark gray opaque powder.

The d -values of the three strongest lines are: 3.157, 2.349, and 2.130 \AA .

Structural data. Dönges [1] in 1951 showed that antimony telluride is isomorphous with bismuth telluride, having the space group $D_{3d}^5-R\bar{3}m$ (No. 166), and $3(\text{Sb}_2\text{Te}_3)$ per unit hexagonal cell, or $1(\text{Sb}_2\text{Te}_3)$ per unit rhombohedral cell. The unit cell measurements reported by Semiletov [2] have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	c
		\AA	\AA
1951	Dönges [1]-----	4.25	30.35
1956	Semiletov [2]-----	4.25	29.92
1963	National Bureau of Standards at 25°C .	4.262	30.450

The density of antimony telluride calculated from NBS lattice constants is 6.513 g/cm^3 at 25°C .

References

- [1] E. Dönges, Über Chalkogenohalogenide des dreiwertigen Antimons und Wismuts. III. Über Tellurohalogenide des dreiwertigen Antimons und Wismuts und über Antimon und Wismut (III)—Tellurid und Wismut (III)—Selenid, Z. anorg. u. Allgem. Chem. **265**, 56–61 (1951).
- [2] S. A. Semiletov, Electronographic determination of antimony telluride structure, Kristallografiya **1**, 403–406 (1956).

hkl (hex.)	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	d	I
	\AA	
003	10.16	1
006	5.08	3
009	3.383	5
104	3.321	1
015	3.157	100
107	2.815	<1
018	2.651	1
1·0·10	2.349	34
0·1·11	2.215	5
110	2.130	23
0·0·15	2.030	4
1·0·13	1.977	4
116	1.964	1
0·1·14	1.875	3
119	1.804	2
205	1.766	10
0·0·18	1.692	2
208	1.661	<1
0·1·17	1.611	2
0·2·10	1.578	7
2·0·11	1.537	1
1·0·19, 1·1·15	1.470	7
0·0·21	1.450	2
0·1·20	1.408	1
125	1.3597	7
1·1·18	1.3249	1
0·0·24, 2·1·10	1.2683	5
0·1·23	1.2462	2
300	1.2303	1
0·2·19	1.2102	2
1·1·21	1.1988	<1
2·0·20, 1·2·14	1.1742	1
1·0·25	1.1563	<1
2·1·16	1.1252	<1
2·0·23	1.0759	<1
220	1.0655	1
2·1·19	1.0522	<1
1·0·28	1.0431	<1
1·2·20	1.0286	<1
0·2·25	1.0167	1
0·1·29	1.0096	1
3·0·18	0.9952	<1
1·3·10	.9704	1
2·2·15	.9434	<1

Arsenic Trioxide, claudetite, As₂O₃ (monoclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of claudetite was obtained from the National Museum, No. 1737 from the San Domingo mines, Portugal. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of aluminum, yttrium, and zinc; 0.01 to 0.1 percent each of barium, calcium, cobalt, chromium, iron, magnesium, titanium, and tungsten.

The sample was colorless. Due to the high indices of refraction a complete optical analysis was not obtained, but partial results seemed to confirm the data given in Dana [4].

The *d*-values of the three strongest lines are: 3.245, 3.454, and 2.771 Å.

Structural data. Buerger [1] in 1942 determined that claudetite has the space group C_{2h}⁵-P2₁/n (No. 14) and 4(As₂O₃) per unit cell.

The density of claudetite calculated from the NBS lattice constants is 4.186 g/cm³ at 25 °C.

References

- [1] M. J. Buerger, The unit cell and space group of claudetite, As₂O₃, Am. Mineralogist **27**, 216 (1942).
- [2] K. A. Becker, K. Plieth, and I. N. Stranski, Strukturuntersuchung der monoklinen Arsenikmodifikation Claudetit, Z. anorg. allgem. Chem. **266**, 293-301 (1951).
- [3] A. J. Frueh, The crystal structure of claudetite (monoclinic As₂O₃) Am. Mineralogist **36**, 833-850 (1951).
- [4] Palache, Berman, and Frondel, Dana's System of Mineralogy, 7th Ed. **1**, 546 (1951).

<i>hkl</i>	Internal Standard Silver, <i>a</i> =4.0861 Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
020	6.496	9
110	4.924	26
011	4.277	4
120	4.118	9
021	3.717	<3
$\bar{1}01$	3.586	14
$\bar{1}11$	3.454	50
130	3.356	20
101	3.328	18
040	3.245	100
031	3.129	5
140	2.771	34
131, 041	2.640	15
210	2.608	14
$\bar{2}11$, 150	2.333	7
002	2.264	24
051	2.253	5
012	2.231	11
221, $\bar{1}51$	2.104	6
151	2.048	5
112, 160	2.005	<3
042	1.857	11
$\bar{1}42$	1.788	4
$\bar{2}51$, 170	1.7514	5
071	1.7163	8
$\bar{1}71$	1.6477	4
080	1.6228	<3
152, $\bar{2}61$	1.5988	<3
180	1.5522	7
$\bar{1}13$	1.4716	4
123	1.3915	<3
$\bar{3}32$, 091	1.3749	4
$\bar{1}82$	1.2937	3
213	1.2667	<3
$\bar{1}63$	1.2220	<3
$\bar{3}72$, 0·11·1	1.1423	<3

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
		Å	Å	Å	
1951	Becker, Plieth and Stranski [2]-----	5.25	12.90	4.53	93°53'
1951	Frueh [3]-----	5.25	12.87	4.54	93°49'
1963	National Bureau of Standards at 25 °C----	5.339 ±. 002	12.984 ±. 001	4.5405 ±. 0005	94°16. 1' ±. 9'

Barium Bromide Monohydrate, BaBr₂·H₂O (orthorhombic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of barium bromide monohydrate was prepared from barium bromide dihydrate obtained from City Chemical Co., New York, N.Y. The hydrate was heated overnight at 85 to 90 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of sodium and strontium; and 0.001 to 0.01 percent each of calcium, magnesium, silicon, and titanium.

The color of the sample was white. The refractive index could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.170, 2.512, and 2.999 Å.

Structural data. Vainstein and Pinsker [1] in 1950 determined that barium bromide monohydrate has the barium chloride monohydrate structure, the space group D_{2h}¹⁶-Pbnm (No. 62), and 4(BaBr₂·H₂O) per unit cell.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		Å	Å	Å
1950	Vainstein and Pinsker [1]----	9.41	11.59	4.59
1963	National Bureau of Standards at 25 °C-----	9.434 ±.001	11.650 ±.001	4.6062 ±.0005

The density of barium bromide monohydrate calculated from the NBS lattice constants is 4.135 g/cm³ at 25 °C.

Reference

[1] B. K. Vainstein and Z. G. Pinsker, Electron diffraction study of BaBr₂·H₂O, Zhur. Fiz. Khim. **24**, 432 (1950).

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
110	7.36	6
020	5.83	23
120	4.96	5
210	4.38	5
101	4.14	12
111	3.91	13
021	3.613	8
121	3.377	2
211	3.170	100
230	2.999	48
040	2.913	18
131	2.836	3
140	2.784	4
301	2.596	14
231	2.512	64
041	2.462	34
400	2.359	26
002	2.303	26
420	2.189	2
022	2.142	3
250, 122	2.091	<2
212	2.038	<2
510	1.863	<2
232	1.827	16
042	1.807	4
061	1.788	11
441	1.703	12
402	1.648	11
270	1.569	9
611	1.476	3
080	1.456	3
213, 512	1.448	6
442	1.434	2
461	1.425	5
081	1.3882	4
303	1.3796	<2
532	1.3658	6
043	1.3582	<2
323, 362	1.3426	<2
272	1.2964	6
343	1.2470	<2
082	1.2308	<2
571, 063	1.2041	3

Barium Stannate, BaSnO₃ (cubic)

Powder data cards

Card number	Index lines	Source
3-0675	2. 91 2. 68 2. 06	H. D. Megaw, Philips Lamps Ltd.

Additional published patterns. None.

NBS sample. The sample of barium stannate was prepared at NBS from stoichiometric amounts of barium carbonate and stannic oxide, pressed into a pellet and heated at 1400 °C for 1 hr. Spectrographic analysis showed the following major impurities: 0.1 percent calcium and 0.01 to 0.1 percent each of aluminum, magnesium, silicon, and strontium.

The sample was very light gray. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 2.911, 1.6805, and 2.058 Å.

Structural data. Megaw [1] in 1946 determined that barium stannate has the perovskite structure, the space group O_h-Pm3m (No. 221), and 1 (BaSnO₃) per unit cell.

Lattice constants

		Å
1946	Megaw [1]-----	4. 1168
1957	Roth [2]-----	4. 114
1958	Wagner and Binder [3]-----	4. 1157
1963	National Bureau of Standards at 25 °C-----	4. 1163

Bismuth Orthophosphate, BiPO₄ (monoclinic)

Powder data cards

Card number	Index lines	Source
1-0812	3. 08 2. 87 4. 20	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. Zemann [2] 1950.

NBS sample. The sample of monoclinic bismuth orthophosphate was obtained from Bios Laboratories, Inc., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of calcium and

The density of barium stannate calculated from the NBS lattice constant is 7.238 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C		
	<i>d</i>	<i>I</i>	<i>a</i>
	Å		Å
110	2. 911	100	4. 117
111	2. 376	4	4. 117
200	2. 058	31	4. 117
211	1. 6805	35	4. 1164
220	1. 4555	16	4. 1167
310	1. 3017	13	4. 1163
222	1. 1882	5	4. 1160
321	1. 1002	13	4. 1166
400	1. 0291	3	4. 1164
411	0. 9702	7	4. 1161
420	. 9204	6	4. 1162
332	. 8776	5	4. 1163
422	. 8402	5	4. 1163
510	. 8073	15	4. 1164
Average value of last five lines-----			4. 1163

References

- [1] H. D. Megaw, Crystal structure of double oxides of the perovskite type, *Proc. Phys. Soc. London* **58**, 133 (1946).
- [2] R. S. Roth, Classification of perovskite and other ABO₃-type compounds, *J. Res. NBS* **58**, 75-88 (1957).
- [3] G. Wagner and H. Binder, The binary systems BaO-SnO₂ and BaO-PbO₂. II. Crystal structure determinations, *Z. anorg. allgem. Chem.* **298**, 12-21 (1958).

sodium and 0.01 to 0.1 percent each of silver, aluminum, copper, iron, magnesium, lead, and silicon.

The color of the sample was white. The indices of refraction could not be obtained because the sample was too fine.

The *d*-values of the three strongest lines are: 3.066, 2.862, and 4.156 Å.

Structural data. Zemann [2] in 1950 determined that monoclinic bismuth orthophosphate has the monazite structure, the space group C_{2h}-P2₁/n (No. 14), with 4(BiPO₄) per unit cell. According to Mooney-Slater [3] 1962, three forms of bismuth phosphate exist: a hexagonal low phase formed from precipitation at room temperature, a high monoclinic phase formed about 700 °C and the monoclinic monazite phase formed above 350 °C.

Bismuth Orthophosphate, BiPO₄ (monoclinic)—Continued

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
1950	Zemann [2]-----	\AA	\AA	\AA	104°
1963	National Bureau of Standards at 25 °C--	6.75 6.752	6.96 6.933	6.42 6.468	103°42.5'

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25 °C	
	<i>d</i>	<i>I</i>
	\AA	
$\bar{1}01$	5.18	8
110	4.761	12
011	4.655	50
$\bar{1}11$	4.156	58
101	4.079	22
111	3.514	23
020	3.466	8
200	3.282	57
002	3.142	13
120	3.066	100
021	3.036	19
210	2.963	19
$\bar{2}11$	2.934	16
012	2.862	73
$\bar{2}02$	2.597	22
211	2.484	3
112	2.438	18
$\bar{2}12$	2.433	16
220	2.382	4
022	2.328	11
130	2.180	3
031	2.170	23
$\bar{1}03$	2.150	23
$\bar{3}11$	2.128	18
$\bar{1}31$	2.112	23
310	2.085	7
131	2.013	5
212	1.959	24
301	1.929	9
$\bar{2}13$	1.916	8

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25 °C	
	<i>d</i>	<i>I</i>
	\AA	
230	1.889	5
$\bar{2}31$	1.882	15
103	1.872	6
032	1.862	20
320	1.850	13
023	1.794	14
$\bar{3}22$	1.755	21
231	1.745	13
040	1.733	14
132	1.729	28
$\bar{3}13$	1.679	5
140	1.676	7
400	1.640	6
$\bar{4}02$	1.620	8
$\bar{3}13$	1.608	3
410	1.596	9
330	1.589	4
312	1.581	7
$\bar{4}12$	1.576	6
240	1.533	15
$\bar{2}14$	1.530	15
042	1.518	3
411	1.467	2
133, 223	1.455	6
242	1.442	4
$\bar{3}14$	1.418	4
421	1.379	7
$\bar{4}31$	1.363	7
303	1.360	3
423	1.355	2
$\bar{5}01$	1.350	5

The density of monoclinic bismuth orthophosphate calculated from NBS lattice constants is 6.863 g/cm³ at 25 °C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-512 (1938).
- [2] J. Zemann, Beitrage zue Kristallchemie des Wismuts, Tschemmaks mineralog. petrog. Mitt. **1**, 361-377 (1950).
- [3] R. C. L. Mooney-Slater, Polymorphic forms of bismuth phosphate, Z. Krist. **117**, 371-385 (1962).

Bismuth Orthophosphate, BiPO₄ (trigonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of trigonal bismuth orthophosphate was precipitated at NBS from a mixture of bismuth nitrate and phosphoric acid. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent sodium and 0.001 to 0.01 percent silicon.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 4.421, 3.025, and 2.854 Å.

Structural data. Mooney-Slater [1] in 1962 determined the structure of the trigonal bismuth orthophosphate; it has the space group D_{3d}^4 -P3₁21 (No. 152) and 3 (BiPO₄) per unit cell. This form is transformed to a monoclinic monazite structure at 350 °C and to another higher temperature monoclinic form above 700 °C.

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1962	Mooney-Slater [1]----	6.966	6.460
1963	National Bureau of Standards at 25 °C	6.9820 ± 0.0004	6.4764 ± 0.0007

The density of trigonal bismuth orthophosphate calculated from NBS lattice constants is 5.538 g/cm³ at 25 °C.

Reference

[1] R.C.L. Mooney-Slater, Polymorphic forms of bismuth phosphate, *Z. Krist.* **117**, 371-385 (1962).

<i>hkl</i>	Internal Standard, Tungsten, <i>a</i> =3.1648 Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
100	6.06	65
101	4.421	100
110	3.494	43
111	3.073	44
200	3.025	94
102	2.854	82
112	2.375	32
210	2.286	12
202	2.211	5
211	2.156	61
103	2.032	6
300	2.016	4
301	1.925	22
212	1.867	51
113	1.837	6
203	1.7571	24
220	1.7452	16
302	1.7115	20
310	1.6774	12
311	1.6239	11
213	1.5693	6
104	1.5644	11
222	1.5368	5
400	1.5118	5
312	1.4892	12
114	1.4687	10
402	1.3698	3
321	1.3563	14
214	1.3206	15
322	1.2750	10
105	1.2667	5
304	1.2624	7
403	1.2384	2
412	1.2217	5
501	1.1885	5
330	1.1639	8
331	1.1450	3
420	1.1425	4
502	1.1328	5
215	1.1267	7
413, 421	1.1255	5
510	1.0860	4
422	1.0774	3
511	1.0709	2

Bismuth Orthovanadate (low form), BiVO_4 (tetragonal)

Powder data cards. None. (Card No. 12-293 gives data for a mineral pucherite, BiVO_4 , which is orthorhombic and does not compare with either of the synthetic forms of BiVO_4 .)

Additional published patterns. None.

NBS sample. The sample of low form bismuth orthovanadate was obtained from City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum and silicon. The sample was also precipitated at NBS from solutions of Na_3VO_4 and $\text{Bi}(\text{NO}_3)_3$. If the precipitate is heated below 400 °C, the tetragonal form is unchanged. Between 400 and 500 °C the changed to the stable monoclinic form occurs.

The color of the sample was orange-yellow. The indices of refraction could not be determined because the sample was too fine.

The d -values of the three strongest lines are: 3.649, 2.738, and 1.879 Å.

Structural data. The structure of low form bismuth orthovanadate has not been reported in the literature. However, because of the similarity of patterns it is thought to be isostructural with zircon, having the space group $D_{4h}^{19}-I4_1/\text{amd}$ (No. 141) and 4(BiVO_4) per unit cell.

Lattice constants

		a	c
		Å	Å
1963	National Bureau of Standards at 26 °C-----	7. 2999	6. 4573

The density of low form bismuth orthovanadate calculated from NBS lattice constants is 6.252 g/cm³ at 26 °C.

hkl	Internal Standard, Tungsten, a 3.1648 Å Cu, 1.5405 Å at 26 °C	
	d	I
	Å	
101	4. 839	47
200	3. 649	100
211	2. 912	22
112	2. 738	61
220	2. 582	21
202	2. 419	3
301	2. 278	18
103	2. 065	11
321	1. 932	14
312	1. 879	48
400	1. 825	15
213	1. 797	7
411	1. 708	5
420	1. 632	11
004	1. 614	7
332	1. 5183	10
204	1. 4765	10
501	1. 4240	6
224	1. 3687	11
521	1. 3261	3
512	1. 3087	12
600	1. 2169	6
404	1. 2092	9
215	1. 2008	5
611	1. 1799	2
532	1. 1673	6
620	1. 1543	7
424	1. 1478	9

Bismuth Orthovanadate (high form), BiVO_4 (monoclinic)

Powder data cards. None. (Card No. 12-293 gives data for a mineral pucherite, BiVO_4 , which is orthorhombic and does not correspond to either form of BiVO_4 which we prepared.)

Additional published patterns. None.

NBS sample. The sample of high form bismuth orthovanadate was prepared by R. S. Roth at NBS by heating stoichiometric mixtures of bismuth oxide and vanadium oxide at 895 °C for 16 hr. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum and silicon. The monoclinic form was also prepared from the low form which was made by precipitation from solutions of Na_3VO_4 and $\text{Bi}(\text{NO}_3)_3$. The low form sample is tetragonal up

to approximately 400 °C. The nonreversible change to the monoclinic form takes place between 400 and 500 °C.

The color of the sample was orange-yellow. The indices of refraction could not be determined because the sample was too fine.

The d -values of the three strongest lines are: 3.095, 3.082, and 3.120 Å.

Structural data. Roth and Waring [1] in 1963 reported that high form BiVO_4 is thought to be isostructural with fergusonite because of the similarity of patterns. Ferguson [2] in 1955 reported that the fergusonite structure is monoclinic. The probable space group is C_{2h}^0-I2/a (No. 15) with 4(BiVO_4) per unit cell.

Bismuth Orthovanadate (high form), BiVO_4 (monoclinic)—Continued

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
		\AA	\AA	\AA	
1963	National Bureau of Standards at 26 °C-----	5.195	11.701	5.092	90.38°

<i>hkl</i>	Internal Standard Silver, $a=4.0861 \text{ \AA}$ Cu, 1.5405 \AA at 26 °C.	
	<i>d</i>	<i>I</i>
	\AA	
020	5.847	2
110	4.749	23
011	4.670	27
130	3.120	32
031, 121	3.095	100
$\bar{1}21$	3.082	96
040	2.924	26
200	2.598	12
002	2.546	14
220	2.374	1
141	2.282	6
$\bar{1}41, 211$	2.277	6
$\bar{2}11$	2.264	11
112	2.250	9
$\bar{1}12$	2.239	7
150	2.133	7
051	2.127	11
231	1.995	5
$\bar{2}31$	1.988	3
132	1.976	5
$\bar{1}32$	1.970	7
060	1.949	4
240	1.943	15
042	1.920	16
202	1.824	6
$\bar{2}02$	1.812	8
$\bar{2}22$	1.726	2
161	1.719	18
$\bar{1}61$	1.717	17
310	1.713	3
013	1.680	3
251	1.648	2
$\bar{2}51$	1.644	3
152	1.639	2
$\bar{1}52$	1.633	2
170	1.591	4
071	1.587	5
330, 321	1.582	10
321	1.5757	9
123	1.5580	8
033	1.5562	4

<i>hkl</i>	Internal Standard Silver, $a=4.0861 \text{ \AA}$ Cu, 1.5405 \AA at 26 °C.	
	<i>d</i>	<i>I</i>
	\AA	
$\bar{1}23$	1.5522	7
062, 242	1.5482	11
242	1.5405	5
080	1.4625	3
$\bar{3}12$	1.4167	2
143, 213	1.4146	2
$\bar{2}13$	1.4067	< 1
053	1.3744	1
$\bar{1}81, 271$	1.3566	2
$\bar{1}72$	1.3481	3
$\bar{3}51$	1.3408	1
262	1.3318	1
400	1.2989	2
280	1.2747	4
004	1.2725	4
082	1.2683	4
091	1.2598	2
361	1.2566	3
$\bar{3}61$	1.2536	4
163	1.2447	3
$\bar{1}63$	1.2417	3
$\bar{3}52, 253$	1.2175	2
$\bar{2}53$	1.2117	1
370	1.2028	1
$\bar{4}31$	1.1958	< 1
073, 323	1.1906	2
440	1.1871	3
323	1.1831	4
044	1.1670	1
402	1.1600	< 1
204	1.1461	1
282	1.1411	1

References

- [1] R. S. Roth and J. L. Waring, Synthesis and stability of bismutotantalite, stibiotantalite, and chemically similar ABO_4 compounds, *Am. Mineralogist* **48**, No. 11, 12, 1348–1356 (1963).
- [2] R. B. Ferguson, The crystallography of synthetic YTaO_4 and fused fergusonite, *Bull. Geol. Soc. Amer.* **66**, 1557 (1955).

The density of high form bismuth orthovanadate calculated from NBS lattice constants is 6.951 g/cm^3 at 26 °C.

Bismuth Telluride (tellurobismuthite), Bi_2Te_3 (trigonal)

Powder data cards

Card number	Index lines	Source
8-21	3. 22 2. 37 2. 19	Thompson [1].
10-54	2. 03 3. 20 3. 25	Vasenin and Konovalov [2].

Additional published patterns. Harcourt [3] 1942.

NBS sample. The sample of bismuth telluride was obtained as a single crystal from Semitronics Inc., Winchester, Mass. Spectrographic analysis showed the following impurities: 0.0001 to 0.001 percent each of magnesium and silicon.

<i>hkl</i> (hex.)	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
003	10. 16	3
006	5. 078	7
101	3. 767	3
104	3. 398	<1
015	3. 222	100
018	2. 689	2
1·0·10	2. 376	26
0·1·11	2. 238	4
110	2. 192	24
113	2. 142	1
0·0·15	2. 031	5
116	2. 113	4
1·0·13	1. 995	2
0·1·14	1. 890	<1
205	1. 812	8
1·0·16	1. 702	2
0·0·18	1. 693	<1
0·2·10	1. 611	6
2·0·11	1. 565	<1
1·1·15	1. 4901	7
0·2·13	1. 4756	1
0·0·21	1. 4513	<1
0·1·20	1. 4140	3
125	1. 3970	6
0·2·16	1. 3449	1
1·1·18	1. 3404	<1
2·1·10	1. 2986	3
300	1. 2660	2
0·1·23	1. 2514	<1
2·1·13	1. 2242	<1
1·1·21	1. 2103	<1
2·0·20	1. 1886	<1
1·0·25	1. 1610	<1
2·1·16	1. 1464	<1
0·1·26	1. 1201	<1

The sample was a gray opaque powder.

The *d*-values of the three strongest lines are: 3.222, 2.376, and 2.192 \AA .

Structural data. Lange [4] in 1939 determined that bismuth telluride has the tetradymite structure with the space group $D_{3d}^5\text{-R}\bar{3}m$ (No. 166) and $3(\text{Bi}_2\text{Te}_3)$ per unit hexagonal cell.

Lattice constants

		<i>a</i>	<i>c</i>
		\AA	\AA
1940	Fronzel [5]-----	4. 39	30. 7
1940	Peacock and Berry [6]--	4. 384	30. 45
1951	Dönges [7]-----	4. 35	30. 3
1954	Semiletov [8]-----	4. 39	30. 46
1963	National Bureau of Standards at 25°C --	4. 3852	30. 483

The density of bismuth telluride calculated from the NBS lattice constants is 7.857 g/cm^3 at 25°C .

<i>hkl</i> (hex.)	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
220	1. 0963	<1
2·0·23	1. 0868	<1
3·0·15	1. 0744	<1
1·0·28	1. 0464	<1
315	1. 0379	<1
0·2·25	1. 0261	<1
0·0·30	1. 0163	<1
2·0·26	. 9978	<1
1·3·10	. 9956	2
1·2·23	. 9738	<1
2·2·15	. 9649	<1
3·0·21	. 9540	<1
1·0·31	. 9518	<1
0·2·28	. 9444	<1
045	. 9382	<1
2·1·25	. 9294	<1
0·1·32, 0·0·33	. 9238	<1
1·2·26, 3·1·17	. 9080	<1
4·0·10	. 9064	<1
2·2·21	. 8750	<1
2·1·28	. 8673	2
3·1·20	. 8666	<1
235	. 8626	<1
1·1·33	. 8512	<1
0·1·35	. 8488	<1
3·2·10	. 8377	<1
410	. 8286	<1

Bismuth Telluride (tellurobismuthite), Bi_2Te_3 (trigonal)—Continued

References

- [1] R. M. Thompson, The telluride minerals and their occurrence in Canada, *Am. Mineralogist* **34**, 342-382 (1949).
- [2] F. I. Vasenin and P. F. Konovalov, Ionization x-ray structure investigation of bismuth telluride, *J. Tech. Phys.* **26**, part 7, 1376 (1956).
- [3] G. A. Harcourt, Tables for the identification of ore minerals by x-ray powder diffraction, *Am. Mineralogist* **27**, 100 (1942).
- [4] P. W. Lange, Ein vergleich zwischen Bi_2Te_3 und $\text{Bi}_2\text{Te}_2\text{S}$, *Naturwissenschaften* **27**, 133 (1939).
- [5] C. Frondel, Redefinition of tellurobismuthite and vandiestite, *Am. J. Sci.* **238**, 880-888 (1940).
- [6] M. A. Peacock and L. G. Berry, Röntgenographic observations on ore minerals, Univ. Toronto Studies Geol. Ser. **44-48**, 67 (1940-1943).
- [7] E. Dönges, Über Chalkogenohalogenide dreiwertigen Antimons und Wismuts III. Über Tellurohalogenide des dreiwertigen Antimons und Wismuts und über Antimon und Wismut III-Tellurid und Wismut III-Selenid, *Z. anorg. allgem. Chem.* **265**, 56 (1951).
- [8] S. A. Semiletov, An electron diffraction study of films of Bi-Se and Bi-Te prepared by evaporation, *Trudy Inst. Krist. Akad. Nauk SSSR* **10**, 76-83 (1954).

Bismuth Trioxide (bismite), $\alpha \text{Bi}_2\text{O}_3$ (pseudo-orthorhombic)

Powder data cards.

Card numbers	Index lines	Source
6-0294	3. 26 1. 96 1. 75	Sillén [1] 1941.
6-0307	3. 23 2. 68 1. 67	Frondel [2] 1943.

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
120	5. 276	2
111	4. 498	4
200	4. 084	4
031	3. 622	8
220	3. 517	2
040	3. 456	19
131	3. 310	33
211	3. 253	100
140	3. 184	25
102	2. 753	6
231	2. 708	38
022	2. 693	39
240	2. 638	6
122	2. 559	15
320	2. 532	9
051	2. 499	7
311	2. 429	6
151	2. 390	14
222	2. 244	6
331	2. 176	6
142	2. 154	5
340	2. 138	2
251	2. 132	8
400	2. 041	2
260	2. 0064	5
302	1. 9922	4
242, 420	1. 9584	26
013	1. 9317	<1
322	1. 9136	2
411	1. 9098	4
113	1. 8787	9
071	1. 8720	17
351	1. 8409	6
171	1. 8237	7
062	1. 8087	1
033	1. 7967	<1
431	1. 7790	2
162	1. 7660	8
360	1. 7590	9
133	1. 7549	6

NBS sample. The sample of bismuth trioxide was obtained from Johnson, Matthey, and Co., Ltd. Their spectrographic analysis showed the following major impurities: less than 0.001 percent each of silicon aluminum, lead, silver, and sodium.

The color of the sample was light yellow. The refractive indices were too high to be determined by the usual liquid-grain immersion method.

The *d*-values of the three strongest lines are: 3.253, 2.693, and 2.708 \AA .

Structural data. Sillén [1] in 1941 determined that alpha bismuth oxide is monoclinic or pseudo-orthorhombic having the monoclinic space group $C_{2h}^5\text{-P}2_1/c$ (No. 14), with $4(\text{Bi}_2\text{O}_3)$ per unit monoclinic cell, or $8(\text{Bi}_2\text{O}_3)$ per unit pseudo-orthorhombic cell. According to Sillén [1], the monoclinic indices *hkl* are transformed into the pseudo-orthorhombic indices *h'k'l'* by the following relations

$$h' = h, k' = k, (\pm) l' = 2l - h$$

The lattice constants reported by Sillén have been converted from kX to angstrom units for comparison with the NBS values.

Bismuth Trioxide (bismite), alpha Bi₂O₃ (pseudo-orthorhombic)—Continued

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
213	1. 7452	16
342	1. 7265	12
180	1. 6914	1
402	1. 6743	13
262	1. 6551	10
233	1. 6431	10
422	1. 6273	2
053	1. 5935	8
280	1. 5920	10
451	1. 5815	7
313	1. 5754	3
153, 511	1. 5632	6
442	1. 5065	6
333	1. 4994	5
531	1. 4888	5
091	1. 4854	6
004	1. 4625	5
104	1. 4391	1
124	1. 4093	3
282	1. 3983	6
073	1. 3882	1
471	1. 3792	3
551	1. 3672	4
1·10·0	1. 3637	3
433	1. 3485	3
044	1. 3462	3

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		Å	Å	Å
1941	Sillén [1]-----	8. 16	13. 81	5. 84
1963	National Bureau of Standards at 25 °C-----	8. 166	13. 827	5. 850

The density of alpha bismuth trioxide calculated from NBS lattice constants is 9.371 g/cm³ at 25 °C.

References

- [1] L. G. Sillén, On the crystal structure of monoclinic α -Bi₂O₃, Z. Krist. **103**, 274-290 (1941).
- [2] C. Frondel, Mineralogy of the oxides and carbonates of bismuth, Am. Mineralogist **28**, Nos. 9 and 10, 521-535 (1943).

Cadmium Perchlorate Hexahydrate, $\text{Cd}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (trigonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of cadmium perchlorate hexahydrate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.0001 to 0.001 percent each of lead and silicon.

The sample was colorless and optically negative with indices of refraction $N_o=1.490$ and $N_e=1.479$.

The d -values of the three strongest lines are: 3.995, 4.223, and 2.902 Å.

Structural data. West [1] in 1935 reported that cadmium perchlorate hexahydrate is trigonal, the space group C_{3v}^1 -P3ml (No. 156) with $1[\text{Cd}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}]$ per unit cell. West reported that the structure is very similar to the hexagonal magnesium perchlorate structure. Moss, Russell, and Sharp [2] confirmed West's determinations. The value of " a " reported by West has been divided by 2 as he suggested. The unit cell values reported by West have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		Å	Å
1935	West [1]-----	7. 92	5. 30
1963	National Bureau of Standards at 25 °C--	7. 9939	5. 3304

The density of cadmium perchlorate hexahydrate calculated from the NBS lattice constants is 2.361 g/cm³ at 25 °C.

References

- [1] C. D. West, The crystal structures of hydrated compounds. II. Structure type $\text{Mg}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$, Z. Krist. **A91**, 480-493 (1935).
- [2] K. C. Moss, D. R. Russell, and D. W. A. Sharp, The lattice constants of some metal fluoroborate hexahydrates, Acta Cryst. **14**, 330 (1961).

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
100	6. 921	25
001	5. 326	17
101	4. 223	75
110	3. 995	100
200	3. 463	4
111	3. 197	51
201	2. 902	66
002	2. 667	2
210	2. 617	1
102	2. 489	18
211	2. 350	25
300	2. 309	9
112	2. 217	7
301	2. 117	26
202	2. 1119	27
220	1. 9985	19
310	1. 9201	8
212	1. 8670	37
311	1. 8064	9
003	1. 7771	3
302	1. 7446	6
103	1. 7205	7
401	1. 6463	4
113	1. 6231	3
320	1. 5880	4
203	1. 5808	9
312	1. 5577	5
321	1. 5223	6
410	1. 5107	6
213	1. 4700	5
411	1. 4539	11
402	1. 4519	11
303	1. 4078	2
322	1. 3642	3
501	1. 3402	4
004, 330	1. 3325	4
420	1. 3082	2
313	1. 3042	5
421	1. 2705	4
114	1. 2641	4
204	1. 2438	3
403	1. 2400	3
502	1. 2287	2
511	1. 2107	5
214	1. 1872	2
323	1. 1841	3
422	1. 1743	3
600	1. 1537	3
413	1. 1510	3
512	1. 1270	3
224	1. 1088	3

Cadmium Sulfate, CdSO₄ (orthorhombic)

Powder data cards

Card number	Index lines	Source
3-0453	3. 30 2. 97 2. 35	Dow Chemical company.

Additional published patterns. None.

NBS sample. The sample of cadmium sulfate was prepared at NBS from cadmium carbonate treated with an excess of sulfuric acid and heated to dryness. Spectrographic analysis showed the major impurities to be 0.001 to 0.01 percent each of aluminum and silicon.

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
001	4. 701	17
110	3. 826	41
101	3. 329	100
020	3. 277	79
111	2. 961	68
021	2. 688	6
200	2. 358	35
002	2. 352	32
121	2. 336	37
012	2. 212	24
201	2. 1044	26
211	2. 0068	18
031	1. 9827	22
220	1. 9155	21
131	1. 8273	17
122	1. 7704	19
202	1. 6648	3
040	1. 6391	12
212	1. 6135	18
032	1. 6004	11
041	1. 5485	3
310	1. 5290	8
013	1. 5250	7
231	1. 5179	7
301	1. 4908	6
222	1. 4843	4
141	1. 4704	9
311	1. 4537	7
113	1. 4497	17
321	1. 3571	11
240	1. 3459	6
232	1. 3243	9
302, 203	1. 3059	4
142	1. 2934	8
051, 150	1. 2634	1
331	1. 2317	7
133	1. 2293	11
151	1. 2204	5

The sample was white. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.329, 3.277, and 2.961 \AA .

Structural data. Kokkoros and Rentzeperis [1] in 1961 determined cadmium sulfate is orthorhombic with the most probable space group D_{2h}^{13} -Pmmn (No. 59) with $2(\text{CdSO}_4)$ per unit cell.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		\AA	\AA	\AA
1961	Kokkoros and Rentzeperis [1].	4. 709	6. 562	4. 694
1963	National Bureau of Standards at 25°C .	4. 7174	6. 5590	4. 7012

The density of cadmium sulfate calculated from NBS lattice constants is 4.759 g/cm^3 at 25°C .

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
322	1. 2140	6
223	1. 2127	4
400	1. 1794	3
014	1. 1570	3
052	1. 1454	5
114	1. 1235	3
251	1. 1136	3
420, 303	1. 1100	3
024	1. 1062	5
341	1. 1032	4
313	1. 0943	6
060	1. 0933	5
421	1. 0798	2
124	1. 0777	2
204	1. 0519	4
412	1. 0407	7
161	1. 0387	6
252	1. 0305	3
342	1. 0221	2
134	1. 0113	3
224	1. 0016	3
260	0. 9918	3
333	. 9897	5
351, 153	. 9839	4
261	. 9702	3
440	. 9576	3
044	. 9552	4
432	. 9498	5

Reference

- [1] P. A. Kokkoros and P. J. Rentzeperis, X-ray investigation of the anhydrous cadmium and mercuric sulphates, *Acta Cryst.* **14**, 329-330 (1961).

Cadmium Telluride, CdTe (cubic)

Powder data cards

Card Number	Index Lines	Source
10-207	3. 74 2. 29 1. 95	Vaughan [1].

Additional published patterns. None.

NBS sample. The sample of cadmium telluride was obtained from Semi-Elements Inc., Saxonburg, Pa. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon and 0.0001 to 0.001 percent each of barium, iron, and lead.

The sample was a black opaque powder.

The *d*-values of the three strongest lines are: 3.741, 2.290, and 1.954 Å.

Structural data. Zachariasen [2] in 1926 determined that cadmium telluride has the zinc sulfide structure, the space group $T_d^2-F\bar{4}3m$ (No. 216), and 4(CdTe) per unit cell. The lattice constants of Zachariasen and Goldschmidt have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constant

		Å
1926	Zachariasen [2].....	6. 477
1926	Goldschmidt [3].....	6. 453
1963	National Bureau of Standards at 25 °C.....	6. 481

The density of cadmium telluride calculated from the NBS lattice constant is 5.856 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C		
	<i>d</i>	<i>I</i>	<i>a</i>
	Å		Å
111	3. 742	100	6. 481
220	2. 290	62	6. 479
311	1. 954	28	6. 482
400	1. 619	5	6. 476
331	1. 488	9	6. 484
422	1. 323	10	6. 482
511	1. 247	4	6. 481
440	1. 146	2	6. 480
531	1. 095	4	6. 479
620	1. 025	4	6. 481
533	0. 9884	2	6. 481
444	. 9356	< 1	6. 482
711	. 9076	2	6. 481
642	. 8661	3	6. 481
731	. 8438	3	6. 482
Average value of last five lines-----			6. 481

References

- [1] D. A. Vaughan, Battelle Memorial Institute, Columbus, Ohio.
- [2] W. H. Zachariasen, Über die Kristallstruktur der Telluride von Beryllium, Zink, Cadmium, und Quecksilber, Z. physik Chem. **124**, 277 (1926).
- [3] V. M. Goldschmidt, Geochemische Verteilungsgesetze der Elemente VII Die Gesetze der Krystallochemie, Skrifter Norske Videnskaps-Akad. Oslo, I: Mat.—Naturv. Kl. No. 2 (1926).

Calcium Fluoride Phosphate (fluorapatite), $\text{Ca}_5\text{F}(\text{PO}_4)_3$ (hexagonal)

Powder data cards

Card number	Index lines	Source
3-0736	2. 81 2. 71 1. 84	McConnell [4] 1937.
12-261	2. 82 2. 72 2. 26	Carobbi and Mazzi [13] 1959.

Additional published patterns. Náray-Szabó [2] 1930, Bale [6] 1940.

NBS sample. The sample of calcium fluoride phosphate was prepared at NBS by J. H. deGroot. A mixture of calcium fluoride and tricalcium orthophosphate was heated in a covered platinum dish to 1250 °C. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent each of magnesium and sodium; and 0.01 to 0.1 percent each of aluminum, barium, germanium, iron, silicon, and strontium.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25 °C	
	<i>d</i>	<i>I</i>
	\AA	
100	8. 12	8
101	5. 25	4
110	4. 684	< 1
200	4. 055	8
111	3. 872	8
201	3. 494	< 1
002	3. 442	42
102	3. 167	13
210	3. 067	17
211	2. 800	100
112	2. 772	54
300	2. 702	62
202	2. 624	29
301	2. 517	6
212	2. 289	7
310	2. 250	22
221	2. 218	3
311	2. 140	6
302	2. 128	3
113	2. 061	5
400	2. 028	1
203	1. 997	4
222	1. 937	26
312	1. 884	14
320	1. 862	4
213	1. 837	32
321	1. 797	15
410	1. 771	13
402	1. 748	13
004	1. 722	15
104	1. 684	< 1
322	1. 637	6
313	1. 607	3
501	1. 580	1
330	1. 562	< 1
420	1. 534	5
331	1. 524	4
214	1. 501	4
421	1. 497	4
502	1. 468	8
510	1. 457	4
304	1. 452	7
323	1. 446	6

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25 °C	
	<i>d</i>	<i>I</i>
	\AA	
511	1. 426	5
332	1. 422	4
413	1. 4015	2
512	1. 3418	2
430	1. 3336	< 1
431	1. 3095	3
520	1. 2995	2
521	1. 2763	3
423	1. 2748	2
324	1. 2635	< 1
215	1. 2560	3
432	1. 2438	2
610	1. 2372	4
414	1. 2341	6
305	1. 2271	9
611	1. 2176	4
522	1. 2154	3
504	1. 1805	< 1
315	1. 1743	< 1
440	1. 1709	1
334	1. 1563	2
433	1. 1532	3
006	1. 1474	1
424	1. 1448	2
106	1. 1359	< 1
523	1. 1306	< 1
116	1. 1144	3
514	1. 1118	2
325	1. 1069	2
702, 532	1. 0984	5
710, 216	1. 0745	< 1
622	1. 0694	< 1
524	1. 0368	< 1
703, 533	1. 0346	< 1
335	1. 0326	2
226	1. 0303	2
712	1. 0257	2
630, 316	1. 0221	2
800	1. 0140	1
631	1. 0110	1
614	1. 0047	1
406	0. 9986	< 1

Calcium Fluoride Phosphate (fluorapatite), $\text{Ca}_5\text{F}(\text{PO}_4)_3$ (hexagonal)—Continued

The sample was colorless and optically negative with the indices of refraction $N_o=1.633$ and $N_e=1.628$.

The d -values of the three strongest lines are: 2.800, 2.702, and 2.772 Å.

Structural data. Hentschel [1] in 1923 determined that fluorapatite has the space group $C_{6h}^2\text{-P6/m}$ (No. 176) and $2[\text{Ca}_5\text{F}(\text{PO}_4)_3]$ per unit cell.

The density of synthetic fluorapatite calculated from the NBS lattice constants is 3.201 g/cm³ at 25 °C.

Lattice constants

		a	c
		Å	Å
1923	Hentschel [1]-----	{9.33	6.83
		{9.43	6.89
1930	Náray-Szabó [2]-----	9.39	6.89
1931	Mehmel [3]-----	9.38	6.86
1939	Thewlis, Glock, and Murray [5]-----	9.38	6.88
1940	Bale [6]-----	9.39	6.89
1941	Klement and Dihn [7]-----	9.38	6.89
1946	Beevers and MacIntyre [8]-----	9.39	6.89
1950	Wallaeys and Chaudron [9]-----	9.350	6.870
1952	Brasseur [10]-----	9.364	6.879
1952	McConnell [11]-----	9.395	6.882
1952	Altschuler, Cisney and Barlow [12]-----	9.386	6.878
1959	Carobbi and Mazzi [13]-----	9.424	6.888
1963	National Bureau of Standards synthetic sample described above.	*9.3684	*6.8841 at 25 °C
	Sample from Durango, Mex. ^a -----	9.3923	6.8821 at 25 °C
	Sample from Llallagua, Bolivia. ^b -----	9.3712	6.8824 at 26 °C

*The error in these values was ± 0.0003 .

^{a, b} These samples were obtained from the National Museum; the number of the Mexican sample is 104021, of the Bolivian sample 103869. These cell constants were derived from powder diffraction measurements made at the same time as those on the synthetic sample.

^a This particular sample from Durango may not be typical because of its lanthanum content. Spectrographic analysis showed 1 to 4 percent of lanthanum and 0.1 to 1.0 percent each of cerium and sodium as major impurities. The error on these lattice constants was ± 0.0005 .

^b Spectrographic analysis showed major impurities to be 0.1 to 1.0 percent of manganese and 0.01 to 0.1 percent each of iron and strontium.

References

- [1] H. Hentschel, Röntgenographische Untersuchungen am Apatit, Centr. Mineral. Geol. p. 609 (1923).
- [2] St. Náray-Szabó, The structure of apatite $(\text{CaF})\text{Ca}_4(\text{PO}_4)_3$, Z. Krist. **75**, 387–398 (1930).
- [3] M. Mehmel, Beziehungen zwischen kristallstruktur und chemischer formel des apatits, Z. physik Chem. **B15**, 223–41 (1931).
- [4] D. McConnell, The substitution of SiO_4 - and SO_4 -groups for PO_4 - groups in the apatite structure; elletadite, the end-member, Am. Mineralogist **22**, 981 (1937).
- [5] J. Thewlis, G. E. Glock, and M. M. Murray, Chemical and x-Ray analysis of dental, mineral, and synthetic apatites, Trans. Faraday Soc. **35**, 358–63 (1939).
- [6] W. F. Bale, A comparative roentgen-ray diffraction study of several natural apatites and the apatite-like constituent of bone and tooth substance, Am. J. Roentgenol. **43**, 735–47 (1940).
- [7] R. Klement and P. Dihn, Isomorphe Apatitarten, Naturwissenschaften **29**, 301 (1941).
- [8] C. A. Beevers and D. B. MacIntyre, The atomic structure of fluorapatite and its relation to that of tooth and bone material, Mineralog. Mag. **27**, 254 (1946).
- [9] R. Wallaeys and G. Chaudron, Sur la preparation de certaines apatites mixtes, Compt. rend. **231**, 355–357 (1950).
- [10] H. Brasseur, Note sur les constantes reticulaires et les indices de refraction des fluor-, chlor-, et hydroxylapatites, Proceedings of the International Symposium on the reactivity of solids, Gothenburg Part 1, 363–7 (1952).
- [11] D. McConnell, The Problem of the carbonate apatites IV, Structural substitutions involving CO_3 and OH, Bull. Soc. Frane. Mineral. et Crist. **75**, 428 (1952).
- [12] Z. S. Altschuler, E. A. Cisney, and I. H. Barlow, X-Ray evidence of the nature of carbonate-apatite, Bull. Geol. Soc. Amer. **63**, 1230–31 (1952).
- [13] G. Carobbi and F. Mazzi, Sulla possibilita di una sostituzione parziale del calcio con l'uranio nel reticolo dell' apatite, Atti. accad. naz. Lincei, Mem. Classe Sci. Fis. Mat. Nat. Ser. II^a [8] **5**, 159–71 (1959).

Cerium Niobium Titanium Oxide (eschynite), CeNbTiO_6 (orthorhombic)

Powder data cards. None.

Additional published patterns. Komkov [1] 1959.

NBS sample. The sample of cerium niobium titanium oxide was prepared at NBS by R. S. Roth from stoichiometric mixtures of cerium oxide, niobium oxide, and titanium oxide. The sample was heated first at 1300 °C for 3 hrs. and then reheated at 1325 °C for three more hours. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and silicon.

The sample was a dark brown opaque powder.

The d -values of the three strongest lines are: 2.975, 3.024, and 3.106 Å.

Structural data. Komkov [1] in 1959 determined that cerium niobium titanium oxide has the space group D_{2h}^{16} -Pmnb (No. 62) with $4(\text{CeNbTiO}_6)$ per unit cell. The lattice constants reported by Komkov have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	b	c
		Å	Å	Å
1959	Komkov [1]-----	7.56	10.99	5.43
1963	National Bureau of Standards at 26°C.	7.538	10.958	5.396

The density of cerium niobium titanium oxide calculated from NBS lattice constants is 5.617 g/cm³ at 26 °C.

Reference

- [1] A. I. Komkov, Minerals of the series euxenite-polycrase and priorite-blomstrandite, Dokl. Akad. Nauk SSSR **126**, 641-644 (1959).

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 26 °C	
	d	I
	Å	
020	5.48	24
011	4.841	5
120	4.431	24
101	4.390	10
111	4.075	13
021	3.847	4
200	3.773	5
121	3.427	4
220	3.106	36
031	3.024	80
211	2.975	100
131	2.808	22
002	2.698	28
140	2.574	10
112	2.474	7
041	2.443	7
122	2.306	9
320	2.283	8
301	2.278	9
240	2.215	9
032	2.170	7
132	2.085	8
222	2.037	25
051	2.031	19
151	1.961	26
331	1.933	11
042	1.922	5
400	1.885	22
142	1.862	9
340	1.852	9
060	1.827	2
312	1.813	2
420	1.783	4
160, 013	1.775	7
341, 103	1.750	4
322	1.744	6
242	1.712	19
123	1.667	6
260	1.643	5
033	1.614	8
213	1.606	13
431	1.600	22
351	1.579	17
223	1.556	7
440	1.553	10
252	1.551	10
402	1.545	10
412	1.528	3
342	1.526	4
043, 071	1.503	7
162	1.483	4
360	1.477	4
143, 171	1.474	4

Cesium Chromate, Cs₂CrO₄ (orthorhombic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium chromate was obtained from the Fairmount Chemical Co. Inc., Newark, N.J. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent rubidium; 0.01 to 0.1 percent each of potassium and sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, and silicon.

The color of the sample was yellow and it is optically positive. The refractive indices are $N_\alpha=1.750$, $N_\beta=1.753$, and $N_\gamma=1.762$.

The d -values of the three strongest lines are: 3.342, 3.207, and 3.364 Å.

Structural data. Miller [1] in 1938 determined that cesium chromate has the potassium sulfate structure, the space group D_{2h}^{16} -Pnam (No. 62) with 4(Cs₂CrO₄) per unit cell.

The lattice constants reported by Miller have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	b	c
		Å	Å	Å
1938	Miller [1]-----	8.380	11.157	6.239
1963	National Bureau of Standards	8.429	11.190	6.302
	25 °C-----	±0.001	±0.001	±0.001

The density of cesium chromate calculated from the NBS lattice constants is 4.266 g/cm³ at 25 °C.

Reference

[1] J. J. Miller, The structure of Cs₂CrO₄, Z. Krist. **99A**, 32-37 (1938).

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
120	4.66	8
111	4.602	9
200	4.213	8
210	3.946	20
121	3.749	69
201	3.505	18
130	3.411	21
220	3.364	77
211	3.342	100
031	3.207	87
002	3.150	66
131	2.998	8
221	2.969	17
230	2.794	24
310	2.725	34
140	2.654	11
122	2.611	15
231	2.554	6
311	2.501	6
212	2.463	17
141	2.449	17
321, 240	2.331	13
132	2.314	31
222	2.301	29
330	2.244	13
241	2.186	8
150	2.163	15
051, 400	2.109	10
232	2.090	15
312	2.062	15
113	2.004	10
401	1.999	9
340	1.982	7
250	1.977	10
420	1.971	14
411	1.967	8
123	1.9152	8
341	1.8911	26
242	1.8743	7
060	1.8653	6
213	1.8542	13
430	1.8349	6
033	1.8308	19
332	1.8280	8
152	1.7833	16
431	1.7615	4
402	1.7521	11
161	1.7499	6
260	1.7060	4
143	1.6474	7
441	1.6263	6

Cesium Fluoride, CsF (cubic)

Powder data cards

Card number	Index lines	Source
1-0872	3. 00 2. 12 3. 48	Davey [1] 1923.

Additional published patterns. None.

NBS sample. The sample of cesium fluoride was obtained from Semi-Elements Inc., Saxonburg, Pa. X-ray patterns were prepared from samples maintained in dry air because of the deliquescence. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent potassium; and 0.001 to 0.01 percent each of aluminum, calcium, copper, iron, lithium, magnesium, nickel, silicon, and sodium. The amount of rubidium impurity was not determined. The sample was colorless.

The *d*-values of the three strongest lines are: 3.003, 3.469, and 2.125 Å.

Structural data. Posnjak and Wyckoff [2] in 1922 determined that cesium fluoride has the sodium chloride structure, the space group O_h^F Fm3m (No. 225), and 4(CsF) per unit cell. The unit cell measurements reported by Davey, Posnjak, and Wyckoff, have been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		Å
1922	Posnjak and Wyckoff [2]-----	6. 04
1923	Davey [1]-----	6. 020
1963	National Bureau of Standards at 25 °C.	6. 014

The density of cesium fluoride calculated from the NBS lattice constant is 4.638 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C		
	<i>d</i>	<i>I</i>	<i>a</i>
	Å		Å
111	3. 469	81	6. 008
200	3. 003	100	6. 007
220	2. 125	37	6. 011
311	1. 8131	25	6. 013
222	1. 7366	10	6. 016
400	1. 5036	7	6. 014
331	1. 3798	6	6. 014
420	1. 3446	10	6. 013
422	1. 2278	5	6. 015
511	1. 1576	4	6. 015
440	1. 0630	2	6. 013
531	1. 0166	3	6. 014
600	1. 0024	3	6. 014
620	0. 9512	4	6. 016
533	. 9173	1	6. 015
622	. 9067	2	6. 014
711	. 8420	2	6. 013
642	. 8036	1	6. 014
731	. 7830	2	6. 014
Average value of last five lines-----			6. 014

References

- [1] W. P. Davey, Precision measurements of crystals of the alkali halides, *Phys. Rev.* **21**, 143-61 (1923).
- [2] E. Posnjak and R. W. G. Wyckoff, The crystal structures of the alkali halides II, *J. Wash. Acad. Sci.* **12**, 248-51 (1922).

Cobalt Fluosilicate Hexahydrate, $\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}$ (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of cobalt fluosilicate hexahydrate was obtained from the City Chemical Co., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, copper, magnesium, nickel, and sodium; and 0.001 to 0.01 percent each of calcium, iron, and manganese.

The color of the sample was pink. The indices of refraction were too low to be measured by the usual liquid grain immersion method.

The d -values of the three strongest lines are: 4.69, 4.18, and 2.595 Å.

Structural data. Hassel and Richter-Salvesen [1] in 1927 determined that cobalt fluosilicate hexahydrate has the nickel chlorostannate structure, the space group $C_{3v}^5\text{-}R3m$ (No. 160), and $1[\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}]$ per unit rhombohedral cell, or $3[\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}]$ per unit hexagonal cell. The unit cell measurements of Hassel and Richter-Salvesen have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		Å	Å
1927	Hassel and Richter-Salvesen [1]-----	9.35	9.69
1962	National Bureau of Standards at 25 °C--	9.370	9.732

The density of cobalt fluosilicate hexahydrate calculated from the NBS lattice constants is 2.081 g/cm³ at 25 °C.

hkl (hex.)	Internal Standard, Tungsten, $a_0 = 3.1648$ Å Co, 1.7889 Å at 25 °C	
	d	I
	Å	
110	4.69	100
102	4.18	63
202	3.116	5
211	2.927	11
113	2.668	5
122	2.595	29
104	2.331	2
311	2.193	3
024	2.086	6
303	2.078	
312	2.042	< 2
401	1.986	3
214	1.907	12
223	1.900	
042	1.872	5
321	1.829	< 2
410	1.771	4
232	1.738	3
134	1.652	7
330	1.562	< 2
413	1.555	< 2
502	1.540	< 2
324	1.479	2
422	1.462	< 2
152	1.397	2
306	1.3916	2
600	1.3524	< 2
226	1.3335	< 2
520	1.2993	5
244	1.2969	4
342	1.2868	2
018	1.2028	< 2
416	1.1963	< 2
440	1.1712	< 2
532, 072	1.1279	< 2

Reference

- [1] O. Hassel and J. Richter-Salvesen, Über den Kristallbau der trigonal kristallisierenden heteropolaren Verbindungen von der Zusammensetzung MG_6LR_6 und $\text{MG}_5\text{D.LR}_6$ und $\text{MG}_4\text{D}_2\text{LR}_6$, Z. physik. Chem. **128**, 345-361 (1927).

Cobalt Perchlorate Hexahydrate, $\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (hexagonal)

Powder data cards. None.

Additional published patterns. West [1] 1935.

NBS sample. The sample of cobalt perchlorate hexahydrate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent of nickel, and 0.001 to 0.01 percent each of copper, magnesium, and silicon.

The color of the sample was pink. It is optically negative with the indices of refraction $N_e=1.492$ and $N_o=1.512$.

The d -values of the three strongest lines are: 3.900, 4.139, and 2.840 Å.

Structural data. West [1] in 1935 determined that cobalt perchlorate hexahydrate has the magnesium perchlorate hexahydrate structure, the space group D_{6h}^{16} -P6/mmm (No. 191), and $4[\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}]$ per unit cell. The lattice constants of West have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
		Å	Å
1935	West [1]-----	15.55	5.21
1963	National Bureau of Standards at 26 °C.	15.610 ±.002	5.2372 ±.0007

The density of cobalt perchlorate hexahydrate calculated from the NBS lattice constants is $2.199 \pm 0.001 \text{ g/cm}^3$ at 26 °C.

hkl	Internal Standard, Silver, $a=4.0861$ Å Co, 1.7889 Å at 26 °C	
	d	I
	Å	
200	6.763	3
101	4.881	4
111	4.345	3
201	4.139	62
220	3.900	100
211	3.661	2
311	3.052	<2
401	2.840	60
002	2.618	8
420	2.556	3
202	2.440	3
421	2.296	10
600	2.253	3
402	} 2.069	8
601		
440	1.952	9
620	1.874	2
422	} 1.828	10
441		
621	1.7655	6
203	1.6907	2
640	1.5502	3
641	1.4869	2
820	1.4753	4
802	} 1.4201	2
821		
443	} 1.3011	4
660		
224	1.2413	2

Reference

- [1] C. D. West, The crystal structures of hydrated compounds II. Structure type $\text{Mg}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$, Z. Krist. A **91**, 480 (1935).

Copper Sulfate (chalcocyanite), CuSO_4 (orthorhombic)

Powder data cards

Card number	Index lines	Source
12-779	2. 62 4. 20 3. 55	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published pattern. Pistorius [2] 1960.

NBS sample. The sample of copper sulfate was obtained from the NBS laboratories in Boulder, Colo. The sample was ground and fumed off with sulfuric acid and placed immediately in a dry atmosphere. Special care was necessary to keep it anhydrous. The sample was mounted in a holder which maintained a dry atmosphere while the patterns were run. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, iron, magnesium, and nickel.

The sample was colorless. The indices of refraction could not be obtained because the sample was too fine.

The d -values of the three strongest lines are: 3.549, (2.616 and 2.611), and 4.187 Å.

Structural data. Kokkoros and Rentzeperis [3] in 1958 determined that copper sulfate has the space group D_{2h}^{16} -Pmnb (No. 62) and 4(CuSO_4) per unit cell. Rama Rao [4] in 1961 made refinements on the structure.

Lattice constants

		a	b	c
		Å	Å	Å
1958	Kokkoros & Rentzeperis [3].	6. 69	8. 39	4. 83
1960	Pistorius [2]-----	6. 811	8. 391	4. 791
1963	National Bureau of Standards at 26 °C.	6. 6982 ± 0. 0006	8. 3956 ±. 0006	4. 8291 ±. 0004

The density of copper sulfate calculated from the NBS lattice constants is 3.903 g/cm³ at 26 °C.

hkl	Internal Standard, Silver, $a=4.0861$ Å Cu, 1.5405 Å at 26 °C	
	d	I
	Å	
011	4. 187	77
101	3. 921	6
111	3. 549	100
200	3. 346	3
021	3. 172	4
121	2. 862	2
220	2. 616	95
211	2. 611	
031	2. 421	50
002	2. 416	
012	2. 321	10
221	2. 301	12
022	2. 093	7
301	2. 027	3
140	2. 003	4
320, 311	1. 971	9
231	1. 963	15
222	1. 7749	28
400	1. 6749	12
042	1. 5843	11
013	1. 5806	10
103	1. 5650	2
420	1. 5553	8
151	1. 5436	3
341	1. 4578	< 1
251	1. 4330	22
213	1. 4298	18
060	1. 3996	4
402	1. 3760	12
422	1. 3073	5
303	1. 3056	
342	1. 2919	3
313	1. 2902	
520, 511	1. 2763	4
062	1. 2107	3
004	1. 2075	2
014	1. 1948	2
162	1. 1918	
442	1. 1508	3
413	1. 1496	
214	1. 1258	3
224	1. 0964	4
620, 611	1. 0790	5
433	1. 0721	4
371	1. 0323	< 1
181, 631	1. 0138	1
244	0. 9990	3
622	. 9850	3
462	. 9812	4
424	. 9536	3
282	. 9249	2

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-512 (1938).
- [2] C. W. F. T. Pistorius, Lattice constants and probable space group of anhydrous cupric sulfate (artificial chalcocyanite), Am. Mineralogist **45**, 744-746 (1960).
- [3] P. A. Kokkoros and P. J. Rentzeperis, The crystal structure of the anhydrous sulfates of copper and zinc, Acta Cryst. **11**, 361 (1958).
- [4] B. Rama Rao, A note on the crystal structure of anhydrous copper sulfate, Acta Cryst. **14**, 321 (1961).

Dysprosium Arsenate, DyAsO₄ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of dysprosium arsenate was prepared at NBS from a water solution of dysprosium trichloride and arsenic pentoxide. The sample was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent antimony and 0.001 to 0.01 percent each of calcium, magnesium, lead, and silicon.

The sample is colorless. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.537, 2.669, and 1.8246 Å.

Structural data. Durif and Forrat [1] in 1957 determined that dysprosium arsenate has the zircon structure with the space group D_{4h}¹⁹-I4₁/amd (No. 141) and 4[DyAsO₄] per unit cell.

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1957	Durif and Forrat [1]---	7.09	6.315
1963	National Bureau of Standards at 25 °C.	7.0733 ± 0.0003	6.3133 ± 0.0003

The density of dysprosium arsenate calculated from the NBS lattice constants is 6.338 g/cm³ at 25 °C.

Reference

- [1] A. Durif and F. Forrat, Sur quelques arsénates des terres rares à structure zircon, *Compt. Rend.* **245**, 1636-38 (1957).

<i>hkl</i>	Internal Standard, Silver, <i>a</i> =4.0861 Å Co, 1.7889 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
101	4.713	15
200	3.537	100
211	2.828	3
112	2.669	67
220	2.500	22
301	2.209	8
103	2.017	8
321	1.873	5
312	1.8246	47
400	1.7681	14
213	1.7522	3
411	1.6556	<3
420	1.5812	14
303	1.5702	4
332	1.4740	14
204	1.4413	12
501	1.3802	<3
224	1.3345	
512	1.2701	10
440	1.2504	<3
600	1.1790	6
404	1.1773	7
532	1.1323	6
424	1.1172	11
631	1.0400	3
116	1.0297	5
415	1.0171	3
444	0.9803	7
552	.9535	9
316	.9521	10
604	.9444	4
624	.9126	9

Erbium Arsenate, ErAsO₄ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of erbium arsenate was prepared at NBS from a water solution of arsenic pentoxide and erbium trichloride. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of nickel and antimony and 0.001 to 0.01 percent each of aluminum, calcium, magnesium, lead, and silicon.

The sample was very pale pink. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.510, 2.652, and 1.812 Å.

Structural data. Durif and Forrat [1] in 1957 determined that erbium arsenate has the zircon structure with the space group D_{4h}¹⁹-I₄/amd (No. 141) and 4(ErAsO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1957	Durif and Forrat [1]-----	7.04	6.30
1963	National Bureau of Standards at 25 °C.	7.0203 ±.0002	6.2761 ±.0004

The density of erbium arsenate calculated from the NBS lattice constants is 6.574 g/cm³ at 25 °C.

Reference

- [1] A. Durif and F. Forrat, Sur quelques arsénates des terres rares à structure zircon, *Compt. Rend.* **245**, 1636-38 (1957).

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648$ Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
101	4.679	12
200	3.510	100
211	2.805	4
112	2.652	68
220	2.481	20
202	2.339	2
301	2.193	8
103	2.005	5
321	1.859	7
312	1.812	52
400	1.755	14
213	1.741	4
411	1.643	2
420	1.5698	15
332	1.4638	14
204	1.4328	9
501	1.3702	1
224	1.3264	8
512	1.2610	10
440	1.2411	3
600, 404	1.1701	7
532	1.1240	7
620, 424	1.1098	12
116	1.0234	3
613	1.0109	< 1
640, 444	0.9734	6
712, 316	.9465	11
604	.9380	4
624	.9062	5
732	.8845	5
800	.8777	< 1
820	.8516	< 1
516	.8329	4
660	.8274	5
752	.7898	10

Europium Arsenate, EuAsO_4 (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of europium arsenate was prepared at NBS from a water solution of arsenic pentoxide and europium trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of antimony and silicon; 0.001 to 0.01 percent each of aluminum, calcium, iron, magnesium, and titanium.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d -values of the three strongest lines are: 3.578, 2.704, and 1.8467 Å

Structural data. No reference to the structure of europium arsenate was found but it is apparently isostructural with yttrium arsenate with the space group D_{4h}^{19} -I $_4$ /amd (No. 141) and 4(EuAsO_4) per unit cell.

Lattice Constants

		a	c
		Å	Å
1963	National Bureau of Standards at 25 °C.	7.1541 ±.0004	6.3953 ±.0004

The density of europium arsenate calculated from the NBS lattice constants is 5.902 g/cm³ at 25 °C.

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Co, 1.7889 Å at 25 °C	
	d	I
	Å	
101	4.77	2
200	3.578	100
112	2.704	63
220	2.530	17
202	2.386	5
301	2.236	5
103	2.0430	3
321	1.8953	5
312	1.8467	45
400	1.7886	12
420	1.5997	11
332	1.4914	12
204	1.4595	8
224	1.3511	8
512	1.2847	8
440	1.2646	3
600, 404	1.1921	7
532	1.1455	8
424	1.1308	10
116	1.0428	5
444	0.9919	5
316	.9643	11
604	.9557	3
624	.9233	6

Gallium Arsenide, GaAs (cubic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of gallium arsenide was obtained from Semitronics Inc., Winchester, Mass. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent iron, 0.01 to 0.1 percent chromium, nickel, and lead; and 0.001 to 0.01 percent each of cobalt, copper, indium, manganese, molybdenum, and silicon.

The sample was a dark gray opaque powder.

The d -values of the three strongest lines are: 3.262, 1.998, and 1.704 Å.

Structural data. Goldschmidt [1] in 1927 determined that gallium arsenide has the zinc sulfide structure, the space group $T_d^2-F\bar{4}3m$ (No. 216), and 4(GaAs) per unit cell.

Lattice constant

1963	National Bureau of Standards at 25 °C-----	Å 5. 652
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The density of gallium arsenide calculated from the NBS lattice constant is 5.321 g/cm³ at 25 °C.

hkl	Internal Standard, Tungsten, $a_s=3.1648$ Å Cu, 1.5405 Å at 25 °C		
	d	I	a
	Å		Å
111	3. 262	100	5. 648
220	1. 998	61	5. 650
311	1. 704	29	5. 650
400	1. 413	7	5. 648
331	1. 297	11	5. 652
422	1. 154	17	5. 647
511	1. 088	5	5. 648
440	0. 9993	3	5. 652
531	. 9557	6	5. 653
620	. 8938	6	5. 652
533	. 8621	4	5. 652
444	. 8159	2	5. 652
711	. 7916	6	5. 652
Average value of last five lines-----			5. 652

Reference

- [1] V. M. Goldschmidt, Geochemische Verteilungsgesetze VIII, Skrifter Norske Vidensk. Akad. Oslo, Math. Nat. K1. 8, 390 (1926-27).

Holmium Arsenate, HoAsO₄ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of holmium arsenate was prepared at NBS from a water solution of arsenic pentoxide and holmium trichloride. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent antimony and 0.001 to 0.01 percent each of aluminum, calcium, iron, lead, and silicon.

The color of the sample was very pale pinkish white. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.528, 2.668, and 1.822 Å.

Structural data. The structure of holmium arsenate was not found in the literature; however, it is apparently isostructural with erbium arsenate having the space group D_{4h}¹⁹-I4₁/amd (No. 141) and 4 (HoAsO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1963	National Bureau of Standards at 25 °C.	7.0548 ±.0003	6.3159 ±.0005

The density of holmium arsenate calculated from NBS lattice constants is 6.420 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, $a_s=3.1648$ Å Cu 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
101	4.709	5
200	3.528	100
211	2.819	4
112	2.668	67
220	2.494	20
202	2.352	6
301	2.203	7
103	2.017	5
321	1.868	4
312	1.822	50
400	1.763	16
420	1.5774	14
332	1.4710	15
204	1.4411	9
501	1.3769	1
224	1.3339	9
413	1.3279	4
512	1.2670	9
440	1.2470	3
404, 600	1.1763	5
532	1.1299	6
424	1.1159	10
116	1.0301	3
206	1.0086	1
640	0.9781	4
552	.9516	7
604	.9428	2
624	.9110	3
732	.8890	4
800	.8818	<1
820	.8556	1
516	.8378	2
644	.8317	3
660	.8314	2

Indium Arsenide, InAs (cubic)

Powder data cards

Card number	Index lines	Source
8-387	1. 24 1. 02 2. 10	Liu and Peretti [1] 1953.

Additional published patterns. A. Iandelli [2] 1941.

NBS sample. The sample of indium arsenide was obtained from Semitronics, Inc., Winchester Mass. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silver, aluminum, bismuth, chromium, iron, gallium, and titanium; and 0.001 to 0.01 percent each of barium, calcium, cobalt, magnesium, nickel, antimony, and tin.

The sample was an opaque metallic powder. The d -values of the three strongest lines are: 3.498, 2.142, and 1.8263 Å.

Structural data. Iandelli [2] in 1941 determined that indium arsenide has the zinc sulfide structure, the space group $T_d^2-F\bar{4}3m$ (No. 216), and 4(InAs) per unit cell. The unit cell measurement reported by Iandelli has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		Å
1941	Iandelli [2]-----	6. 048
1953	Liu and Peretti [1]-----	6. 058
1963	National Bureau of Standards at 25 °C-----	6. 058

The density of indium arsenide calculated from NBS lattice constant is 5.668 g/cm³ at 25 °C.

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C		
	d	I	a
	Å		Å
111	3. 498	100	6. 059
200	3. 030	8	6. 060
220	2. 142	61	6. 059
311	1. 8263	38	6. 057
222	1. 7489	2	6. 058
400	1. 5145	9	6. 058
331	1. 3895	13	6. 057
420	1. 3544	2	6. 057
422	1. 2366	15	6. 058
511	1. 1658	9	6. 058
440	1. 0707	7	6. 057
531	1. 0241	10	6. 058
600	1. 0097	1	6. 058
620	0. 9578	6	6. 058
533	. 9239	3	6. 058
444	. 8745	3	6. 059
711	. 8483	6	6. 058
642	. 8096	15	6. 058
731	. 7887	8	6. 058
Average value of last five lines-----6. 058			

References

- [1] T. S. Liu and E. A. Peretti, The indium-arsenic system, Trans. Am. Soc. Metals **45**, 677-85 (1953).
- [2] A. Iandelli, Sulla struttura dei composti, InP, InAs, e InSb, Gazz. chim. ital. **71**, 58-62 (1941).

Lanthanum Arsenate, LaAsO₄ (monoclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of lanthanum arsenate was prepared at NBS from a water solution of arsenic pentoxide and lanthanum trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, iron, and silicon, and 0.001 to 0.01 percent each of calcium, magnesium, lead, and antimony.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.185, 2.983, and 3.391 Å.

Structural data. No reference to the structure of lanthanum arsenate was found; however, it is apparently isostructural with lanthanum phosphate with the space group C_{2h}⁵-P_{21/n} (No. 14) and 4(LaAsO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
		Å	Å	Å	
1963	National Bureau of Standards at 25 °C.	7.0078 ±. 0007	7.212 ±. 001	6.7670 ±. 0007	104°29.3' ±. 6'

The density of lanthanum arsenate calculated from the NBS lattice constants is 5.572 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Silver, <i>a</i> =4.0861 Å Cu, 1.5405 Å at 25 °C		<i>hkl</i>	Internal Standard, Silver, <i>a</i> =4.0861 Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>		<i>d</i>	<i>I</i>
	Å			Å	
101	5.45	4	322	1.832	20
110	4.95	12	231, 223	1.808	6
011	4.85	10	040	1.803	5
111	4.35	8	132	1.795	22
101	4.215	<1	140, 321	1.743	11
111	3.635	7	400	1.696	4
020	3.606	16	402	1.689	7
200	3.391	60	410	1.651	11
002	3.278	8	330, 114	1.647	11
120	3.185	100	004	1.638	5
210	3.068	24	312	1.632	4
012	2.983	87	214	1.604	7
202	2.722	24	332, 240	1.593	8
212	2.546	22	142	1.581	2
112	2.527	15	124	1.531	6
220	2.471	6	322	1.519	2
122	2.430	8	411	1.516	1
301	2.326	6	413	1.504	2
031	2.257	11	242	1.502	2
103	2.252	10	314	1.487	3
311	2.213	7	341, 421	1.425	2
221	2.185	6	431, 423	1.416	4
122, 310	2.159	3	340	1.410	3
013, 131	2.089	4	124, 043	1.391	9
212	2.023	31	134	1.383	8
301	1.991	3	332, 511	1.374	9
231	1.959	5	204, 412	1.348	4
103, 132	1.942	32	414	1.337	6
320	1.916	14	510	1.333	3
023	1.868	4	052	1.320	8

Lanthanum Niobium Titanium Oxide, LaNbTiO₆ (monoclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of lanthanum niobium titanium oxide was prepared at NBS by R. S. Roth from stoichiometric mixtures of the oxides of lanthanum, niobium, and titanium. The sample was first heated at 1300 °C for 3 hr and then heated at 1350 °C for 3 hr. Spectrographic analysis of the original oxides showed no impurities greater than 0.05 percent.

The sample was colorless. The refractive indices could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.444, 3.331, and 3.306 Å.

Structural data. P. M. de Wolff [1] in 1962 determined that lanthanum niobium titanium oxide has a C-centered monoclinic lattice.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
		Å	Å	Å	
1962	de Wolff [1]	11.20	8.85	5.27	115°18'
1963	National Bureau of Standards at 25 °C.	11.196	8.851	5.265	115°16'

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648$ Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
110	6.68	22
200	5.063	10
111	4.523	10
111	3.444	100
220	3.331	100
311	3.306	94
021	3.241	36
221	3.183	16
310	3.153	10
130	2.833	11
202	2.632	31
131	2.573	30
400	2.531	20
312	2.421	6
421	2.355	8
331	2.273	14
311	2.249	4
330	2.223	10
511	2.170	6
022	2.096	9
112	2.065	12
422	2.033	16
041	2.006	10
241	1.993	8
132	1.941	8

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648$ Å Cu 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
332	1.916	4
202	1.868	10
331	1.825	10
531	1.783	31
241	1.761	16
150	1.744	10
441	1.731	9
222	1.721	10
621	1.715	8
151	1.678	6
530	1.669	9
113	1.651	6
042, 223	1.620	10
511	1.603	11
620	1.579	4
711	1.563	5
333	1.507	9
152	1.459	4
531	1.427	4

Reference

[1] P. M. de Wolff, private communication.

Lithium Phosphate, low form (lithiophosphate), Li_3PO_4 (orthorhombic)

Powder data cards

Card number	Index lines	Source
12-230	3. 98 3. 80 2. 67	Fisher [1] 1958.

A high form is obtained from samples that have been heated above approximately 500 °C.

Additional published pattern. Matias and Bondareva [2] 1957.

NBS sample. The sample of lithium phosphate was obtained from the City Chemical Co., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent calcium; 0.01 to 0.1 percent each of aluminum, sodium, and strontium; and 0.001 to 0.01 percent each of barium, iron, magnesium, and silicon.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The d -values of the three strongest lines are: 3.973, 3.797, and 2.640 Å.

Structural data. Zemmann [3] in 1960 studied a crystal of Li_3PO_4 that had been grown in molten LiCl and determined that it has the space group D_{2h}^{16} -Pmnb (No. 62) and $4(\text{Li}_3\text{PO}_4)$ per unit cell. We find that the lower form apparently has the same structure with only slight changes in the lattice constants, principally in the c -direction. The cell constants of Zambonini and Laves have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
		Å	Å	Å
1932	Zambonini and Laves [4].	6. 08	10. 28	4. 87
1963	National Bureau of Standards at 25 °C.	6. 1155 ±. 0004	10. 467 ±. 001	4. 8452 ±. 0005

References

- [1] D. J. Fisher, Note on lithiophosphate, *Am. Mineralogist* **43**, 761-2 (1958).
- [2] V. V. Matias and A. M. Bondareva, Lithiophosphate, a new mineral, *Doklady Akad. Nauk S.S.S.R.* **112**, 124-6 (1957); an English abstract exists in *Am. Mineralogist* **42**, 585 (1957).
- [3] J. Zemmann, Die Kristallstruktur von Lithiumphosphat, Li_3PO_4 , *Acta Cryst.* **13**, 863-7 (1960).
- [4] F. Zambonini and F. Laves, Über die Kristallstruktur des Li_3PO_4 und seine Beziehung Zum Strukturtyp des Olivin, *Z. Krist.* **83**, 26-28 (1932).

The density of lithium phosphate, low form, calculated from the NBS lattice constants is 2.480 g/cm³ at 25 °C.

hkl	Internal Standard Silver, $a=4.0861$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
020	5. 232	34
120	3. 973	100
101	3. 797	98
021	3. 554	56
121	3. 071	} 26
200	3. 059	
220	2. 640	64
040	2. 616	36
002	2. 423	47
221	2. 318	} 31
041	2. 303	
022	2. 199	<1
141	2. 155	4
122	2. 070	3
320, 202	1. 899	1
301	1. 879	2
241	1. 839	4
222	1. 785	14
321	1. 769	9
142	1. 7074	1
160	1. 6777	2
061	1. 6415	1
340	1. 6083	3
161	1. 5855	2
103	1. 5616	4
023, 312	1. 5431	3
400	1. 5287	11
260	1. 5152	16
123	1. 4959	1
420	1. 4675	1
421	1. 4043	2
223	1. 3776	14
143	1. 3409	2
440	1. 3203	2
080	1. 3078	<1
402	1. 2931	4
262	1. 2848	8
053, 361	1. 2788	4
303	1. 2656	2
422	1. 2550	1
243	1. 2533	1
280	1. 2027	<1
520	1. 1909	2
501	1. 1860	2
281	1. 1676	3
442	1. 1591	2
460	1. 1498	<1
343	1. 1394	<1
380	1. 1014	2

Lithium Phosphate, high form, Li_3PO_4 (orthorhombic)

Powder data cards. None. Powder data card No. 12-230 has a pattern by Fisher [1] which seems to be for the low form. The sample is changed to the high form when it has been heated above approximately 500 °C.

Additional published patterns. Tien and Hummel [2], 1961.

NBS sample. The sample of lithium phosphate was obtained from the City Chemical Co, New York, N.Y. It was heated at 800 °C for 15 min.

Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent calcium; 0.01 to 0.1 percent each of aluminum, sodium, and strontium; and 0.001 to 0.01 percent each of barium, iron, magnesium, and silicon.

The sample was colorless and optically positive, with the indices of refraction $N_\alpha=1.550$, $N_\beta=1.556$, and $N_\gamma=1.560$.

The d -values of the three strongest lines are: 3.978, 3.834 and 2.640 Å.

<i>hkl</i>	Internal Standard, Tungsten, $a_s=3.1648$ Å Cu 1.5405 Å at 25 °C		<i>hkl</i>	Internal Standard, Tungsten, $a_s=3.1648$ Å Cu 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>		<i>d</i>	<i>I</i>
	Å			Å	
020	5.24	29	171	1.3943	<1
011	4.46	7	162	1.3873	<1
120	3.978	100	143	1.3562	<1
101	3.834	93	431	1.3467	<1
021, 111	3.588	63	233	1.3361	2
121	3.093	18	440	1.3198	1
200	3.058	17	080	1.3095	<1
220	2.640	67	402	1.2984	5
040	2.619	37	262	1.2910	8
131	2.583	27	180, 361	1.2806	5
311	2.521	14	313	1.2682	4
002	2.462	47	081	1.2651	2
140	2.406	3	323	1.2414	<1
221	2.327	3	181	1.2390	<1
041	2.313	4	333	1.2002	4
141	2.163	2	520, 253	1.1905	3
122	2.095	6	501	1.1875	2
231	2.084	5	163	1.1731	2
051	1.927	3	281	1.1688	3
212	1.885	<1	034	1.1608	1
311	1.853	5	460	1.1499	<1
241	1.844	4	182, 214	1.1354	<1
151	1.838	4	531	1.1231	<1
222	1.800	14	380	1.1015	2
042	1.793	5	234	1.0850	1
321	1.772	6	522	1.0719	<1
060	1.745	<1	314	1.0481	1
160	1.679	3	154	1.0456	<1
331	1.657	4	363	1.0314	<1
061	1.646	2	064, 382	1.0056	1
251	1.6305	1	2·10·0	0.9910	<1
340	1.6080	3	391	.9902	<1
103	1.5848	4	453	.9867	<1
023	1.5659	5	472, 503, 621	.9805	<1
341, 400	1.5285	9	481	.9749	<1
260	1.5158	17	283, 552	.9705	<1
420	1.4673	1	533	.9442	<1
133	1.4429	7	602, 354	.9414	<1
213, 332, 071	1.4322	5			
421	1.4067	<1			

Structural data. Zemann [3] in 1960 studied a crystal of Li_3PO_4 that had been grown in molten LiCl and determined that it has the space group D_{2h}^{16} -Pmnb (No. 62) and $4(\text{Li}_3\text{PO}_4)$ per unit cell. The cell constants of Zambonini and Laves have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		Å	Å	Å
1932	Zambonini and Laves [4].	6.08	10.28	4.87
1960	Zemann [3]-----	6.12	10.53	4.93
1963	National Bureau of Standards at 25° C.	6.1147 ±.0005	10.475 ±.001	4.9228 ±.0005

The density of lithium phosphate, high form, calculated from the NBS lattice constants is 2.439 g/cm³ at 25 °C.

References

- [1] D. J. Fisher, Note on lithiophosphate, *Am. Mineralogist* **43**, 761-2 (1958).
- [2] T. Y. Tien and F. A. Hummel, Studies in lithium oxide systems: X, lithium phosphate compounds, *J. Am. Ceram. Soc.* **44**, 206-8 (1961).
- [3] J. Zemann, Die Kristallstruktur von Lithiumphosphat, Li_3PO_4 , *Acta Cryst.* **13**, 863-7 (1960).
- [4] F. Zambonini and F. Laves, Über die Kristallstruktur des Li_3PO_4 und seine Beziehung Zum Strukturtyp des Olivin, *Z. Krist.* **83**, 26-28 (1932).

Magnesium Ammonium Phosphate Hexahydrate (struvite), $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ (orthorhombic)

Powder data cards

Card number	Index lines	Source
5-0316	4. 28 2. 93 2. 69	Hanawalt, Rinn and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of struvite was precipitated at NBS from a solution of magnesium sulfate by adding a solution of ammonium monohydrogen orthophosphate. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent sodium, and 0.001 to 0.01 percent each of calcium, iron, and silicon.

The sample was colorless and optically positive. The indices of refraction are $N_\alpha=1.493$, $N_\beta=1.496$, and $N_\gamma=1.501$.

The d -values of the three strongest lines are: 4.257, 5.601, and 2.919 Å.

Structural data. Bland and Basinski [2] in 1959 determined that struvite has the space group C_{2v}^7 - $\text{Pm}2_1$ n (No. 31) and $2(\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O})$ per unit cell.

Lattice constants

		a	b	c
		Å	Å	Å
1944	Palache, Berman and Frondel [3]	6. 10	11. 20	6. 97
1959	Bland and Basinski [2]	6. 13	11. 19	6. 92
1963	National Bureau of Standards at 25 °C	6. 945 ±. 001	11. 208 ±. 002	6. 1355 ±. 0008

The density calculated from the NBS lattice constants is 1.706 g/cm³ at 25 °C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, Ind. Eng. Chem., Anal. Ed. **10**, 457-512 (1938).
- [2] J. A. Bland and S. J. Basinski, Crystal symmetry of struvite (guanite), Nature **183**, 1385-7 (1959).
- [3] C. Palache, H. Berman, and C. Frondel, Dana's System of Mineralogy, 7th Ed. **2**, 715 (1944).

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
001	6. 14	7
110	5. 905	41
020	5. 601	58
011	5. 378	27
101	4. 600	6
111	4. 257	100
021	4. 139	40
121	3. 557	4
200	3. 475	11
130	3. 289	27
031	3. 192	2
002	3. 067	3
201	3. 022	14
012	2. 958	23
211	2. 919	54
040	2. 802	34
112	2. 722	15
022	2. 690	50
221	2. 660	43
041	2. 548	3
122	2. 511	7
141	2. 394	5
231	2. 352	12
202	2. 300	1
212	2. 253	4
240	2. 180	4
301	2. 167	3
150	2. 133	5
222, 311	2. 127	7
042	2. 069	6
241	2. 054	11
003	2. 046	
151	2. 014	10
142	1. 983	5
103, 232	1. 960	14
113	1. 932	2
023	1. 921	3
331	1. 873	5
123	1. 851	3
312	1. 822	3
052	1. 810	8
251	1. 801	14
033	1. 794	10
203	1. 762	9
133, 400	1. 737	14
341	1. 714	5
223	1. 681	4
332	1. 657	4

Potassium Chlorate, KClO_3 (monoclinic)

Powder Data cards

Card number	Index lines	Source
1-0599	3.45 2.79 2.86	Hanawalt, Rinn and Frevel [1] 1938.
12-571	3.46 2.88 2.80	Institute of Physics, University College, Cardiff.

Additional published patterns. None.

NBS sample. The sample of potassium chlorate was obtained from the General Chemical Co., New York, N.Y., and recrystallized to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, barium, iron, rubidium, silicon, sodium, and strontium.

The color of the sample was white. It is optically negative with the indices of refraction $N_\alpha=1.408$, $N_\beta=1.516$, and $N_\gamma=1.524$; $2V$ was very small.

The d -values of the three strongest lines are: 3.45, 3.34, and 2.868 Å.

Structural data. Zachariasen [2] and [3] in 1928 determined that potassium chlorate has the space group $C_{2h}^2 P2_1/m$ (No. 11) and $2[\text{KClO}_3]$ per unit cell. The unit cell measurements of Ieviš and Ozols and Zachariasen have been converted from kX to angstrom units for comparison with the NBS values.

The density of potassium chlorate calculated from the NBS lattice constants is 2.339 g/cm³ at 26 °C.

References

- [1] J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem. Anal. Ed. **10**, 457-513 (1938).
- [2] W. H. Zachariasen, The crystal structure of sesquioxides and compounds of the type ABO_3 , Skrifter Norske Videnskaps-Akad. Oslo I: Mat.-Naturv. Kl. Nr. **4**, 82 (1928).
- [3] W. H. Zachariasen, The crystal structure of potassium chlorate, Z. Krist. **71**, 501 (1929).
- [4] A. Ieviš and J. Ozols, Precision determination of lattice constants of monoclinic crystals, Doklady Akad. Nauk SSSR **91**, 527-30 (1953).

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 26 °C	
	d	I
	Å	
001	6.69	3
$\bar{1}01$	4.41	10
011	4.29	5
110	3.45	100
002	3.34	60
$\bar{1}02$	3.234	3
101	3.204	4
012	2.868	35
020	2.794	33
111	2.779	23
021	2.579	4
120	2.356	3
$\bar{2}01$	2.327	18
102	2.309	2
$\bar{2}11, \bar{1}13$	2.149	6
022	2.145	7
112	2.135	7
$\bar{1}22$	2.115	17
013	2.070	2
$\bar{2}03$	1.919	5
201	1.902	5
$\bar{2}13$	1.815	2
$\bar{2}11$	1.800	1
$\bar{2}21, \bar{1}23$	1.7888	2
122	1.7800	1
$\bar{1}04$	1.7730	<1
103	1.7615	<1
023	1.7421	1
130	1.7149	2
113	1.6800	1
032	1.6279	5
$\bar{1}32$	1.6145	2
131	1.6111	2
014	1.6014	3
$\bar{2}23$	1.5820	<1
221	1.5722	<1
$\bar{2}14$	1.5539	<1
302	1.5428	<1
124	1.4973	4
123	1.4897	4
$\bar{3}11$	1.4848	4
303	1.4700	<1
033	1.4296	1
313	1.4213	2
310	1.4137	<1
040	1.3978	2
203	1.3517	<1
005, $\bar{2}33$	1.3371	1
$\bar{2}15$	1.3254	<1
213	1.3136	<1
$\bar{3}23$	1.3009	2
042	1.2899	<1

Potassium Chlorate, KClO_3 (monoclinic)—Continued

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
		\AA	\AA	\AA	
1929	Zachariasen [3]-----	4. 656	5. 596	7. 099	109°38'
1953	Ieviš and Ozols [4]-----	4. 6569	5. 59089	7. 0991	109°38.9'
1963	National Bureau of Standards at 26 °C-----	4. 6553 ±. 0002	5. 5905 ±. 0006	7. 1006 ±. 0005	109°41.1' ±. 3'

Potassium Lithium Sulfate, KLiSO_4 (hexagonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium lithium sulfate was prepared at NBS by dissolving stoichiometric amounts of solid potassium hydroxide and lithium hydroxide in a small amount of water. When the mixture was at room temperature a drop of 1 percent bromcresol-purple was added and the mixture neutralized with H_2SO_4 . The solution was evaporated to dryness and the precipitate was then heated to about 750 °C to sharpen the pattern. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, indium, and sodium; and 0.001 to 0.01 percent each of aluminum, rubidium, and silicon.

The sample is colorless and optically negative. The indices of refraction are $N_o = 1.471$ and $N_e = 1.469$.

The *d*-values of the three strongest lines are: 3.960, 3.099, and 2.573 Å.

Structural data. Nowacki [1] in 1942 determined that potassium lithium sulfate has the space group $C_6^2\text{-P6}/3$ (No. 173) and $2(\text{KLiSO}_4)$ per unit cell. The lattice constants of Nowacki have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>c</i>
		\AA	\AA
1942	Nowacki [1]-----	5. 14	8. 62
1963	National Bureau of Standards at 26 °C--	5. 1457	8. 6298

The density of potassium lithium sulfate calculated from NBS lattice constants is 2.385 g/cm³ at 26 °C.

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 Å at 26 °C	
	<i>d</i>	<i>I</i>
	\AA	
002	4. 320	12
101	3. 960	100
102	3. 099	70
110	2. 573	34
111	2. 465	16
103	2. 418	5
200	2. 225	8
112	2. 211	20
201, 004	2. 158	19
202	1. 981	12
113	1. 919	4
203	1. 762	2
210	1. 683	3
114, 211	1. 653	11
105	1. 6096	5
212	1. 5690	11
204	1. 5499	4
300	1. 4852	11
213	1. 4533	2
106	1. 3687	2
205	1. 3647	3
214	1. 3276	3
220	1. 2864	5
116	1. 2550	5
222	1. 2329	2
311, 304	1. 2237	6
206	1. 2081	2
215	1. 2055	3
107, 312	1. 1880	3
313	1. 1356	1
401, 224	1. 1048	2
216	1. 0939	1
402	1. 0787	2
108	1. 0484	1
403	1. 0389	1
306	1. 0335	1

Reference

- [1] W. Nowacki, Beziehungen zwischen $\text{K}[\text{AlSiO}_4]$ (Tief-Kaliophililit), $\text{Ba}[\text{Al}_2\text{O}_4]$, $\text{K}[\text{LiSO}_4]$, $\text{Na}[\text{AlSiO}_4]$ (Nephelin) und Si_2O_4 (β -Tridymit), *Naturwissenschaften* **30**, 471-472 (1942).

Potassium Perchromate, K_3CrO_8 (tetragonal)

Powder data cards. None.

Additional published patterns. Wilson [1] 1941.

NBS sample. The sample of potassium perchromate was obtained from City Chemical Corp., New York, N.Y. Spectrographic analysis did not show any impurities greater than the range 0.0001 to 0.001 percent.

The color of the sample was deep red. The indices of refraction are $N_o=1.774$ and $N_e=1.730$. It is optically negative.

The d -values of the three strongest lines are: 2.979, 2.372, and 1.856 Å.

Structural data. Wilson [1] in 1941 determined that potassium perchromate has the space group $D_{2d}^{11}-I4_2m$ (No. 121) and $2(K_3CrO_8)$ per unit cell. Potassium perchromate is used as a structure type. The unit cell measurements reported by Wilson have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		a	c
		Å	Å
1941	Wilson [1]-----	6.71	7.62
1963	National Bureau of Standards at 25 °C.	6.711	7.641

The density of potassium perchromate calculated from NBS lattice constants is 2.869 g/cm³ at 25 °C.

Reference

- [1] I. A. Wilson, X-ray analysis of potassium perchromate, K_2CrO_8 , and isomorphous compounds, Arkiv. Kemi Minerali. Geol. **B15**, 1-7 (1941).

hkl	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1:5405 Å at 25 °C	
	d	I
	Å	
101	5.054	42
110	4.749	18
002	3.822	1
200	3.357	36
112	2.979	100
211	2.795	17
202	2.524	5
220	2.372	53
301	2.147	5
310	2.121	2
222	2.016	7
004	1.911	9
312	1.856	47
321	1.808	7
303, 400	1.677	5
204	1.659	7
330	1.5815	5
402	1.5365	3
420	1.5004	10
224	1.4880	12
332	1.4615	10
314	1.4198	<1
413	1.3718	2
501	1.3219	<1
404	1.2607	6
512	1.2445	10
116, 521	1.2299	5
440	1.1863	4
325	1.1808	4
600	1.1183	2
532	1.1020	3
316	1.0920	2

Potassium Zinc Decavanadate 16 Hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$ (triclinic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium zinc decavanadate 16 hydrate, was obtained from H. T. Evans, Jr., U.S. Geological Survey, Washington, D.C. It was prepared from a solution of potassium metavanadate and zinc acetate in water with the pH adjusted between 3 and 4 with acetic acid. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of aluminum, barium, calcium, chromium, iron, magnesium, molybdenum, lead, and rubidium.

The color of the sample was bright orange. The indices of refraction could not be determined because of imperfections in the crystals.

The d -values of the three strongest lines are: 8.18, 7.40, and 9.45 Å.

Structural data. Evans, Mrose, and Marvin [1], in 1955 determined that potassium zinc decavanadate 16 hydrate, has the space group $C_1^1-P\bar{1}$ (No. 2) and $1(K_2Zn_2V_{10}O_{28} \cdot 16H_2O)$ per unit cell.

The density of potassium zinc decavanadate calculated from the NBS lattice constants is 2.708 g/cm³ at 25 °C.

Reference

- [1] H. T. Evans, Jr., M. E. Mrose, and R. Marvin, Constitution of the natural and artificial decavanadates, *Am. Mineralogist* **40**, 314 (1955).

hkl	Internal Standard, Tungsten $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
010	10.01	23
100	9.45	28
110	8.61	20
001	8.18	100
$\bar{1}\bar{1}1$	7.40	35
$\bar{1}01$	7.17	3
0 $\bar{1}1$	6.81	7
011	5.95	5
101	5.52	6
$\bar{2}\bar{1}1$	5.17	9
020	5.00	14
200	4.72	9
$\bar{2}01$	4.63	4
$\bar{1}\bar{1}1$	4.60	4
$\bar{2}\bar{2}1$	4.53	<1
220	4.33	<1
$\bar{1}02$	4.166	3
002	4.094	16
121	3.960	3
211	3.759	4
$201, \bar{2}\bar{2}\bar{2}$	3.697	7
$\bar{1}31$	3.630	2
202	3.580	3
$\bar{2}\bar{3}1$	3.548	4
$\bar{3}21$	3.487	8
102	3.448	6
022	3.402	3
230	3.373	1
030	3.333	4
112	3.279	2
$\bar{3}01$	3.229	3
$\bar{2}\bar{3}2, 300$	3.149	5
212	3.011	6
022	2.977	3
031	2.951	5
$\bar{3}\bar{3}2, 330$	2.883	3
$0\bar{3}2, \bar{1}23$	2.778	11
003	2.730	14
$\bar{2}03$	2.680	1
$\bar{2}42, \bar{3}41$	2.595	<1
$\bar{3}\bar{1}3$	2.569	2
$222, \bar{1}13$	2.557	2
420	2.525	2
$\bar{1}33, \bar{4}32$	2.485	4
103, 331	2.458	2
$\bar{3}03$	2.389	9
042	2.278	8
$\bar{1}51$	2.164	6
$\bar{3}13$	2.139	8
$\bar{5}32$	2.102	1
$\bar{2}04$	2.085	2
$\bar{2}34$	2.071	1
$2\bar{1}3, \bar{2}\bar{3}2, \bar{1}\bar{5}2$	2.065	<1
$\bar{3}34$	2.046	1
$\bar{1}42, \bar{1}33$	2.006	4
530	1.987	4
043, 033	1.985	4
4 $\bar{1}1$	1.964	1
$\bar{1}33$	1.930	<1

Potassium Zinc Decavanadate 16 Hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$ (triclinic)—Continued

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	α	β	γ
1955	Evans, Mrose and Marvin [1].	$\overset{\text{\AA}}{10.76}$	$\overset{\text{\AA}}{11.17}$	$\overset{\text{\AA}}{8.77}$	$104^\circ 50'$	$109^\circ 29'$	$65^\circ 05'$
1963	National Bureau of Standards at 25 °C.	$10.778 \pm .003$	$11.146 \pm .003$	$8.774 \pm .003$	$104^\circ 57' \pm 1'$	$109^\circ 32' \pm 1'$	$65^\circ 0' \pm 2'$

Rubidium Chromate, Rb_2CrO_4 (orthorhombic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium chromate was obtained from the Fairmount Chemical Co., Inc., Newark, N.J. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent potassium; 0.01 to 0.1 percent sodium; and 0.001 to 0.01 percent each of aluminum, barium, calcium, and silicon.

The color of the sample was yellow and it is optically positive. The refractive indices are $N_\alpha=1.715$, $N_\beta=1.725$, and $N_\gamma=1.759$.

The *d*-values of the three strongest lines are: 3.207, 3.191, and 3.083 Å.

Structural data. Smith and Colby [1] in 1940 determined that rubidium chromate has the potassium sulfate structure and the space group D_{2h}^{16} -Pnam (No. 62) with 4(Rb_2CrO_4) per unit cell.

The lattice constants reported by Smith and Colby have been converted from kX to angstrom units for comparison with NBS values.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		$\overset{\text{\AA}}{\text{Å}}$	$\overset{\text{\AA}}{\text{Å}}$	$\overset{\text{\AA}}{\text{Å}}$
1940	Smith and Colby [1].	7.999	10.726	6.301
1963	National Bureau of Standards at 25° C.	$8.001 \pm .001$	$10.722 \pm .001$	$6.074 \pm .001$

The density of rubidium chromate calculated from NBS lattice constants is 3.657 g/cm³ at 25° C.

Reference

- [1] H. W. Smith, Jr. and M. Y. Colby, The crystal structure of rubidium chromate, Rb_2CrO_4 , Z. Krist. **103**, 90-95 (1940).

<i>hkl</i>	Internal Standard, Tungsten $\alpha=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	$\overset{\text{\AA}}{\text{Å}}$	
020	5.365	1
120	4.451	2
200	4.004	6
210	3.749	14
121	3.593	36
201	3.342	16
130	3.263	18
220	3.207	100
211	3.191	100
031	3.083	95
002	3.037	57
131	2.872	4
221	2.838	13
040	2.680	12
230	2.664	18
022	2.644	3
310	2.588	30
140	2.541	6
122	2.509	11
231	2.442	5
320	2.388	4
311	2.380	14
212	2.359	22
141	2.344	14
240	2.226	25
222	2.205	30
330	2.138	11
241	2.091	7
150	2.071	12
051	2.021	4
042	2.0098	11
232	2.0035	20
400	2.0010	18
312	1.9697	12
401	1.8997	10
340	1.8908	5
420	1.8737	7
411	1.8703	9
123	1.8426	6
341, 251	1.8047	
060	1.7859	6
213	1.7813	13
033	1.7621	15
430	1.7461	10

Silver Antimony Telluride, AgSbTe₂ (cubic)

Powder data cards. None.

Additional published patterns. Geller and Wernick [1] 1959.

NBS sample. The sample of silver antimony telluride was obtained from Semitronics Inc., Winchester, Mass. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of aluminum, bismuth, copper, iron, indium, and tin; and 0.001 to 0.01 percent each of gold, calcium, chromium, magnesium, nickel, and titanium.

The sample was an opaque metallic gray powder.

The *d*-values of the three strongest lines are: 3.042, 2.151, and 1.7554 Å.

Structural data. Geller and Wernick [1] in 1959 determined that silver antimony telluride has the sodium chloride structure, the space group *O*_h⁵—Fm3m (No. 225), and 2(AgSbTe₂) per unit cell.

Lattice constants

		Å
1959	Geller and Wernick [1] at 25 °C	6.078
1963	National Bureau of Standards at 25 °C	6.080

The density of silver antimony telluride calculated from the NBS lattice constant is 7.163 g/cm³ at 25 °C.

Sodium Magnesium Aluminum Boron Hydroxy Silicate, dravite (var. of tourmaline), NaMg₃Al₆B₃Si₆O₂₇(OH)₄ (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of dravite is U.S. National Museum No. 103791 from Dobruva, Carinthia, Austria. This mineral sample was picked by C. R. Robbins, NBS, as a true end member representative of the magnesium rich variety of tourmaline. The chemical analysis by H. B. Wiik, Helsingfors, Westend, Finland, showed the following: 36.99 percent SiO₂; 0.39 percent TiO₂; 32.00 percent Al₂O₃; 0.01 percent MnO; 11.58 percent MgO; 0.50 percent CaO; 0.01 percent Li₂O; 3.11 percent Na₂O; 0.08 percent K₂O; 3.08 percent H₂O⁺; 10.77 percent B₂O₃; 0.25 percent F; and 0.90 percent total Fe as FeO.

The color of the sample was light brown and it is optically negative. The indices of refraction are *N*_o=1.634 and *N*_e=1.613.

The *d*-values of the three strongest lines are: 2.576, 3.985, and 2.961 Å.

<i>hkl</i>	Internal Standard, Tungsten, <i>a</i> =3.1648 Å Cu, 1.5405 Å at 25 °C		
	<i>d</i>	<i>I</i>	<i>a</i>
	Å		Å
111	3.511	1	6.081
200	3.040	100	6.080
220	2.151	65	6.084
311	1.8332	<1	6.080
222	1.7554	19	6.081
400	1.5203	9	6.081
331	1.3946	<1	6.079
420	1.3597	18	6.081
422	1.2411	9	6.079
511	1.1703	<1	6.081
440	1.0748	4	6.080
531	1.0276	<1	6.079
600	1.0133	4	6.080
620	0.9614	3	6.080
622	.9166	2	6.080
444	.8775	1	6.079
711	.8513	<1	6.079
640	.8433	2	6.081
642	.8125	2	6.080
Average value of last five lines			6.080

Reference

- [1] S. Geller and J. H. Wernick, Ternary semiconducting compounds with sodium chloride-like structure: AgSbSe₂, AgSbTe₂, AgBiS₂, AgBiSe₂, Acta Cryst. **12**, 46–54 (1959).

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1948	Hamburger and Buerger [2]	15.951	7.24
1949	Belova and Belova [3]	16.00	7.24
1951	Kurylenko [4]	15.676	7.03
1963	National Bureau of Standards at 25 °C	15.931	7.197

The density of dravite calculated from NBS lattice constants is 3.019 g/cm³ at 25 °C.

**Sodium Magnesium Aluminum Boron Hydroxy Silicate, dravite (var. of tourmaline),
NaMg₃Al₆B₃Si₆O₂₇(OH)₄ (trigonal)—Continued**

<i>hkl</i> (<i>hex</i>)	Internal Standard Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
101	6.377	28
021	4.981	25
300	4.595	17
211	4.221	66
220	3.985	84
012	3.480	62
131	3.375	16
401	3.111	5
410	3.008	12
122	2.961	83
321	2.897	9
330	2.656	<1
312	2.622	7
051	2.576	100
042	2.490	1
241	2.451	1
003	2.396	20
232	2.376	19
511	2.342	21
600	2.300	5
502	2.189	17
431	2.163	14
303	2.127	16
422	2.112	10
223	2.054	21
152	2.040	46
161	2.019	7
440	1.991	5
342	1.920	34
701	1.901	6
413	1.877	7
621	1.849	8
710	1.828	2
612	1.817	2
104	1.784	9

<i>hkl</i> (<i>hex</i>)	Internal Standard Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
333	1.781	7
024	1.742	5
532	1.729	4
541	1.715	2
262	1.690	1
603	1.660	24
271	1.641	16
550	1.592	21
452	1.586	<1
811	1.575	<1
324	1.565	<1
461	1.5456	5
900	1.5326	7
722	1.5262	7
820	1.5056	16
244	1.4807	3
514	1.4555	19
642	1.4485	11
015	1.4318	8
651	1.4178	8
205	1.4091	19
125	1.3871	2
381	1.3746	3
10.0.1	1.3551	9
912	1.3416	5
921	1.3359	4
045	1.3282	13
660, 553	1.3272	12
10.1.0	1.3095	12
571	1.3002	1
903	1.2922	2
505	1.2765	14
425	1.2602	3
155	1.2449	3
0.11.1	1.2358	3
482	1.2260	1
850	1.2149	3

References

- [1] M. J. Buerger and W. Parrish, The unit cell and space group of tourmaline (an example of the inspective equiinclination treatment of trigonal crystals), *Am. Mineralogist* **22**, 1139-1150 (1937).
- [2] G. E. Hamburger and M. J. Buerger, The structure of tourmaline, *Am. Mineralogist* **33**, 532-540 (1948).
- [3] N. V. Belova and E. N. Belova (The crystal structure of tourmaline), *Dokl. Akad. Nauk SSSR* **69**, No. 2, 185-188 (1949).
- [4] C. Kurylenko, Transformation de la dravite de Doubrova (Moravie) de 375° à 1350° , *Compt. rend. Paris* **232**, 2109-2111 (1951).

Sodium Trimetaphosphate, $\text{Na}_3\text{P}_3\text{O}_9$ (orthorhombic)

Powder data cards.

Card number	Index lines	Source
11-648	3. 40 3. 86 3. 04	deWolff, Techn. Phys. Dienst, Delft, Holland.

Additional published patterns. Corbridge and Tromans [1].

NBS sample. The sample of sodium trimetaphosphate was crystallized by heating sodium trimetaphosphate above the melting point (about 650 °C) and then cooling slowly at the rate of 5 to 10 °C an hour. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, potassium, magnesium, silicon, and titanium.

The sample is colorless.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25 °C	
	<i>d</i>	<i>I</i>
	\AA	
110	6. 79	43
011	6. 65	53
111	5. 095	43
021	5. 015	48
121	4. 237	5
200	3. 960	16
002, 130	3. 850	63
131	3. 444	48
211	3. 407	100
112	3. 351	31
022	3. 330	37
221	3. 110	11
041	3. 037	55
141	2. 837	11
202	2. 762	41
132	2. 723	22
212	2. 706	10
310	2. 591	11
240	2. 540	35
013	2. 522	14
150, 051	2. 503	7
311	2. 457	8
241	2. 412	11
113	2. 406	8
151	2. 387	< 1
232, 321	2. 340	< 1
123	2. 292	2
330	2. 267	6
060	2. 204	8
331	2. 175	11

The *d*-values of the three strongest lines are: 3.407, 3.850, and 3.037 Å.

Structural data. Ondik and Gryder [2] in 1960 determined that sodium trimetaphosphate has the space group $C_{2v}^9\text{-P2}_1\text{cn}$ (No. 33) or $D_{2h}^{16}\text{-Pmcn}$ (No. 62) with 4($\text{Na}_3\text{P}_3\text{O}_9$) per unit cell.

<i>hkl</i>	Internal Standard, Tungsten $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25 °C	
	<i>d</i>	<i>I</i>
	\AA	
133	2. 136	8
213	2. 128	10
242	2. 121	8
152	2. 103	2
223	2. 050	10
043	2. 029	17
341	1. 994	6
400	1. 982	9
143	1. 965	5
332	1. 954	6
004, 260	1. 927	5
252	1. 911	8
411, 420	1. 900	1
350	1. 871	13
024	1. 849	10
170	1. 838	4
243	1. 806	4
153	1. 794	2
171	1. 781	1
402	1. 762	1
134	1. 723	1
214	1. 719	< 1
333	1. 699	2
352	1. 681	5
224	1. 675	8
063, 253	1. 671	8
271, 044	1. 665	5
441	1. 661	5
144	1. 629	1
234	1. 612	6
181	1. 583	2
054	1. 557	5
451	1. 554	7
073	1. 521	3
082	1. 518	2
353	1. 511	5
371	1. 507	6
025	1. 501	6
531	1. 465	3
254	1. 449	5
372	1. 427	11
282	1. 418	2

Sodium Trimetaphosphate, $\text{Na}_3\text{P}_3\text{O}_9$ (orthorhombic)—Continued

Lattice constants

The density of sodium trimetaphosphate calculated from the NBS lattice constants is 2.515 g/cm³ at 25 °C.

		<i>a</i>	<i>b</i>	<i>c</i>
		Å	Å	Å
1960	Ondik and Gryder [2].	7.93	13.14	7.75
1962	deWolff-----	7.928	13.22	7.703
1963	National Bureau of Standards at 25 °C.	7.930	13.220	7.705

References

- [1] D. E. C. Corbridge and F. R. Tromans, Identification of sodium phosphates with an x-ray focusing camera, *Anal. Chem.* **30**, 1101-1110 (1958).
- [2] H. M. Ondik and J. W. Gryder, Crystal chemistry of the hydrates of sodium trimetaphosphate, *J. Inorg. Nucl. Chem.* **14**, Nos. 3/4, 240-246 (1960).

Sodium Trimetaphosphate Monohydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$ (orthorhombic)

Powder data cards

Card number	Index lines	Source
1-0977	2.84 3.03 2.60	New Jersey Zinc Co.
11-391	4.96 3.57 3.01	Corbridge and Tromans [1] 1958.

Card number 12-10 also is called $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$; however, it contains a very different pattern, perhaps another form.

Additional published patterns. None.

NBS sample. The sample of sodium trimetaphosphate monohydrate was prepared at NBS by heating sodium dihydrogen orthophosphate for 5 hr at 530 °C. Solid sodium trimetaphosphate was salted out with NaCl and then recrystallized several times. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, potassium, magnesium, silicon, and titanium.

The sample is colorless and it is probably optically negative. The indices of refraction are $N_\alpha=1.493$, $N_\beta=1.502$, and $N_\gamma=1.504$.

The *d*-values of the three strongest lines are: 3.566, 2.825, and (2.605 and 2.601) Å

Structural data. Ondik and Gryder [2] in 1960 determined that sodium trimetaphosphate monohydrate has the space group $C_{2v}^9\text{-P2}_1\text{cn}$ (No. 33) or $D_{2h}^{16}\text{-Pmcn}$ (No. 62) with $4(\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O})$ per unit cell.

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648$ Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
110	7.144	42
011	6.553	38
111	5.195	49
021	4.968	60
121	4.289	32
200	4.252	5
130	3.905	32
002	3.778	17
012	3.633	15
211	3.566	100
131	3.469	64
112	3.340	60
022	3.278	55
221	3.230	8
122	3.060	8
041	3.022	73
141	2.848	5
202	2.825	100
310	2.769	57
212	2.762	
132	2.716	10
240	2.605	75
311	2.601	
150	2.520	5
051	2.491	18
042	2.484	21
013	2.474	
330	2.382	39
113, 232	2.375	6
331	2.272	17
123, 302	2.266	4
312	2.235	4
060	2.198	16
052	2.163	<2
213	2.139	15

Sodium Trimetaphosphate Monohydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$ (orthorhombic)—Continued

Lattice constants

<i>hkl</i>	Internal Standard, Tungsten, $a = 3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
400	2.125	17
133	2.116	12
341	2.067	8
420	2.022	5
332	2.016	10
043	2.001	12
421, 260	1.954	29
143	1.949	12
350	1.930	13
252	1.927	9
062	1.900	6
261, 004	1.889	11
351	1.870	9
162, 431	1.855	4
170, 412	1.840	6
053	1.823	9
024	1.817	7
243, 323	1.811	3
171, 440	1.786	11
153	1.781	10
352	1.719	16
253	1.674	17
413	1.612	10

		<i>a</i>	<i>b</i>	<i>c</i>
		\AA	\AA	\AA
1960	Ondik and Gryder [2].	8.53	13.21	7.58
1963	National Bureau of Standards at 25°C .	8.500 ± 0.001	13.189 ± 0.001	7.558 ± 0.001

The density of sodium trimetaphosphate monohydrate calculated from NBS lattice constants is 2.539 g/cm^3 at 25°C .

References

- [1] D. E. C. Corbridge and F. R. Tromans, Identification of sodium phosphates with an x-ray focusing camera, *Anal. Chem.* **30**, No. 6, 1101-1110 (1958).
- [2] H. Ondik and J. W. Gryder, Crystal chemistry of the hydrates of sodium trimetaphosphate, *J. Inorg. Nucl. Chem.* **14**, 240-246 (1960).

Stannous Fluoride, SnF_2 (monoclinic)

Powder data cards. None

Additional published patterns. Nebergall, Muhler, and Day [1] 1952.

NBS sample. The sample of stannous fluoride was obtained from the Indiana University School of Dentistry, Indianapolis, Ind. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of calcium and silicon.

The sample was colorless. The indices of refraction were not determined because the sample reacted with the index liquids.

The *d*-values of the three strongest lines are: 3.552, 3.200 and 3.379 \AA .

Structural data. Bergerhoff [2] in 1962 determined that stannous fluoride has the space group C_{2h}^6 - $C2/c$ (No. 15) and 16 $[\text{SnF}_2]$ per unit cell.

Difficulties in indexing the NBS pattern were overcome with the help of single crystal work done by Dr. Howard T. Evans Jr., of the U.S. Geological Survey.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>	β
		\AA	\AA	\AA	
1962	Bergerhoff [2]	13.46	4.92	13.86	$109^\circ 30'$
1963	National Bureau of Standards at 25°C	13.353 ± 0.001	4.9089 ± 0.0004	13.787 ± 0.001	$109^\circ 6.5'$ $\pm 3'$

Stannous Fluoride, SnF_2 (monoclinic)—Continued

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
$\bar{1}11$	4.489	5
112	3.552	100
$\bar{2}04$	3.379	40
$\bar{3}11$	3.298	2
$\bar{3}12$	3.200	60
400	3.155	34
$\bar{2}04$	2.571	11
020	2.455	9
021	2.412	1
$\bar{5}11$	2.327	2
$\bar{3}15$	2.320	3
$\bar{3}13$	2.315	2
$\bar{6}02$	2.225	1
$\bar{6}04$	2.109	10
$\bar{2}22$	2.084	<1
$\bar{1}16$	2.059	18
$\bar{3}16$	2.048	2
$\bar{2}24$	1.986	16
512	1.954	16
420	1.938	18
$\bar{5}16$	1.854	12
602	1.833	<1
$\bar{7}12, \bar{2}24$	1.776	22
408	1.690	2
008	1.629	5
$\bar{1}31, \bar{3}16$	1.6186	6
$\bar{6}24$	1.5997	6
800	1.5769	4
132	1.5594	5
604	1.5504	3

The density of stannous fluoride calculated from the NBS lattice constants is 4.875 g/cm^3 at 25°C .

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
332	1.5258	5
$\bar{9}12$	1.4112	<1
$\bar{4}28$	1.3921	4
$\bar{8}08$	1.3812	1
028	1.3570	2
$\bar{9}16$	1.3517	2
$\bar{10} \cdot 0 \cdot 4$	1.3325	1
$\bar{3} \cdot 1 \cdot 10, \bar{1}36, 820$	1.3271	5
$\bar{6}24$	1.3107	2
$\bar{5} \cdot 1 \cdot 10, \bar{8}26, 0 \cdot 0 \cdot 10$	1.3031	<1
532	1.2974	2
408	1.2858	1
$\bar{5}36$	1.2667	2
912	1.2446	1
$\bar{7}32$	1.2411	2
$\bar{7} \cdot 1 \cdot 10, \bar{7}31$	1.2313	2
040, $\bar{7}34$	1.2273	1
$1 \cdot 1 \cdot 10$	1.2153	1
$\bar{8}28$	1.2036	1
336	1.1836	1
$\bar{7}16, \bar{10} \cdot 2 \cdot 4$	1.1712	2
$\bar{11} \cdot 1 \cdot 2$	1.1645	1
$\bar{2}44$	1.1536	1
$0 \cdot 2 \cdot 10, \bar{7} \cdot 1 \cdot 11$	1.1508	<1
440	1.1435	<1
428	1.1387	<1
$\bar{2} \cdot 0 \cdot 12$	1.1335	<1

References

- [1] W. H. Nebergall, J. C. Muhler, and H. G. Day, The preparation and properties of stannous fluoride, *J. Am. Chem. Soc.* **74**, 1604 (1952).
- [2] G. Bergerhoff, Zur Kristallstruktur des Zinn-II-fluorides, *Acta Cryst.* **15**, 509 (1962).

Strontium 1:1 Borate, $\text{SrO} \cdot \text{B}_2\text{O}_3$ (orthorhombic)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of strontium 1:1 borate was prepared at NBS by C. E. Weir. A suspension of hydrogen 3:1 borate (boric acid) and strontium carbonate was evaporated to dryness and heated at 1000 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of barium and silicon; 0.001 to 0.01 percent each of calcium and sodium.

The sample is colorless and optically negative with $N_\alpha=1.632$, $N_\beta=1.650$, and $N_\gamma=1.660$.

The d -values of the three strongest lines are: 3.467, 6.013, and 2.688 Å.

Structural data. Block, Perloff, and Weir [1] in 1963 determined that strontium 1:1 borate has the space group D_{2h}^{14} -Pnca (No. 60) and 4($\text{SrO} \cdot \text{B}_2\text{O}_3$) per unit cell.

Lattice constants

		a	b	c
		Å	Å	Å
1963	Block, Perloff and Weir [1].	6.577	12.02	4.329
1963	National Bureau of Standards at 25 °C.	6.5890 ±.0004	12.018 ±.001	4.3373 ±.0005

The density of strontium 1:1 borate calculated from the NBS lattice constants is 3.350 g/cm³ at 25 °C.

Reference

[1] S. Block, A. Perloff, and C. E. Weir. The crystallography of some M^{+2} borates, *Acta Cryst.* **17**, 314 (1964).

hkl	Internal Standard, Silver, $a=4.0861$ Å Cu, 1.5405 Å at 25 °C	
	d	I
	Å	
020	6.013	69
111	3.467	100
200	3.292	37
210	3.176	47
121	3.101	15
040	3.004	37
220	2.888	40
131	2.688	67
141	2.313	5
240	2.221	30
002	2.169	27
022	2.041	21
060, 151	2.003	58
241	1.977	9
122	1.948	7
311	1.934	44
202	1.812	8
212	1.792	4
331	1.760	23
222	1.734	14
260	1.712	10
400	1.647	<2
420	1.589	11
171, 242	1.5518	21
430	1.5232	5
351	1.5192	
080	1.5023	4
062	1.4712	3
440	1.4447	5
113	1.4020	4
280	1.3667	5
262	1.3434	8
133	1.3320	8
371	1.2911	6
422	1.2820	6
460	1.2724	4
511	1.2543	9
153	1.2174	6
531	1.2027	15
282, 333	1.1564	4
2·10·0	1.1291	<2
551	1.1165	5
480	1.1100	5
391	1.1036	5
600	1.0980	5
173	1.0906	3
620	1.0804	5
1·11·1	1.0461	<2
640	1.0313	<2
571	1.0161	5
2·10·2	1.0013	3
482, 373	0.9879	4

Terbium Arsenate, TbAsO₄ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of terbium arsenate was prepared at NBS from a water solution of arsenic pentoxide and terbium trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent silicon; 0.001 to 0.1 percent each of antimony, calcium, iron, magnesium, and lead.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.550, 2.685, and 1.834 Å.

Structural data. No reference to the structure of terbium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group D_{4h}¹⁹-I4₁/amd (No. 141) and 4(TbAsO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1963	National Bureau of Standards at 25 °C.	7. 1025	6. 3536

The density of terbium arsenate calculated from the NBS lattice constants is 6.172 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, <i>a</i> = 3.1648 Å Co, 1.7889 Å at 25° C	
	<i>d</i>	<i>I</i>
	Å	
101	4. 736	8
200	3. 550	100
112	2. 685	69
220	2. 510	22
202	2. 367	7
301	2. 219	9
103	2. 029	8
321	1. 882	6
312	1. 834	53
400	1. 775	16
420	1. 5878	15
332	1. 4809	14
204	1. 4500	11
224	1. 3423	8
512	1. 2755	13
440	1. 2553	4
600, 404	1. 1838	8
532	1. 1373	8
424	1. 1230	12
116	1. 0364	4
444	0. 9849	5
316	. 9577	7
604	. 9495	3
624	. 9168	5

Thallium Chromate, Tl₂CrO₄ (orthorhombic)

Powder data cards. None.

Additional published patterns. Abbad and Rivoir [1] 1947.

NBS sample. The sample of thallium chromate was prepared at NBS from solutions of thallium nitrate and sodium chromate. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent lead; 0.01 to 0.1 percent each of aluminum and silicon; and 0.001 to 0.01 percent each of barium, calcium, and antimony.

The color of the sample was yellow. The refractive indices could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.145, 3.060, and 3.186 Å.

Structural data. Abbad and Rivoir [1] in 1947 determined that thallium chromate has the potassium sulfate structure, the space group D_{2h}¹⁶-Pnam (No. 62), and 4(Tl₂CrO₄) per unit cell.

The lattice constants reported by Abbad and Rivoir have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		Å	Å	Å
1947	Abbad and Rivoir [1]-----	7. 82	10. 70	5. 92
1963	National Bureau of Standards at 25 °C-----	7. 908	10. 730	5. 913
		±. 001	±. 001	±. 001

The density of thallium chromate calculated from the NBS lattice constants is 6.946 g/cm³ at 25 °C.

Thallium Chromate, Ti_2CrO_4 (orthorhombic)—Continued

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
020	5.37	5
011	5.19	8
120	4.45	12
111	4.337	23
210	3.714	15
121	3.553	54
201	3.290	27
130	3.263	24
220	3.186	57
211	3.145	100
031	3.060	96
002	2.958	53
221	2.805	14
040, 112	2.685	6
230	2.654	16
310	2.561	28
140	2.540	25
122	2.461	15
320	2.366	8
311	2.349	13
141	2.336	10
212	2.314	10
240	2.221	11
321	2.197	15
132	2.191	13
222	2.167	32
330	2.122	9
241	2.079	17
150	2.071	15
051	2.017	4
440	1.977	19
232	1.975	16
151	1.954	6
312	1.936	14
142	1.9270	13
250	1.8863	9
401	1.8750	12
420	1.8553	15
322, 411	1.8472	14
123	1.8013	26
341	1.7921	26
060	1.7885	14
242	1.7755	7
203	1.7640	7
213	1.7409	17

<i>hkl</i>	Internal Standard, Tungsten, $a=3.1648 \text{ \AA}$ Cu, 1.5405 \AA at 25°C	
	<i>d</i>	<i>I</i>
	\AA	
430	1.7305	22
033	1.7259	19
332	1.7235	14
152	1.6963	15
161	1.6726	13
431	1.6603	9
402	1.6434	5
260	1.6294	5
412	1.6250	5
252	1.5903	6
422, 261	1.5713	10
143	1.5573	3
062	1.5299	6
520	1.5167	6
511	1.5125	6
170	1.5045	6
432	1.4931	8
071	1.4837	7
004	1.4782	5
521	1.4696	5
450	1.4539	4
361	1.4355	6
262	1.4271	5
124, 442	1.4020	3
403	1.3959	4
413	1.3842	4
540	1.3623	6
343	1.3602	5
522	1.3498	5
134	1.3462	5
080, 172, } 224 }	1.3410	6
370	1.3250	6
600	1.3182	4

Reference

- [1] M. Abbad and L. Rivoir, La estructura del cromato talioso, Anales Soc. españ. fís. y. quím **43**, 831-836 (1947)

Thulium Arsenate, TmAsO₄ (tetragonal)

Powder data cards. None.

Additional published patterns. None.

NBS sample. The sample of thulium arsenate was prepared at NBS from a water solution of arsenic pentoxide and thulium trichloride. It was dried at 110 °C. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of silicon and antimony; 0.001 to 0.01 percent each of aluminum, calcium, iron, lead, and magnesium.

The sample was colorless. The indices of refraction could not be determined because the sample was too fine.

The *d*-values of the three strongest lines are: 3.497, 2.644, and 1.8064 Å.

Structural data. No reference to the structure of thulium arsenate was found, but it is apparently isostructural with yttrium arsenate with the space group D_{4h}¹⁹-I₄₁/amd (No. 141) and 4(TmAsO₄) per unit cell.

Lattice constants

		<i>a</i>	<i>c</i>
		Å	Å
1963	National Bureau of Standards at 25 °C	6.9939 ± 0.0003	6.2595 ± 0.0003

The density of thulium arsenate calculated from the NBS lattice constants is 6.678 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard, Tungsten, <i>a</i> = 3.1648 Å Cu, 1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
101	4.667	11
200	3.497	100
211	2.796	5
112	2.644	72
220	2.473	23
202	2.333	5
301	2.1851	10
103	1.9993	7
321	1.8524	7
312	1.8064	55
400	1.7483	16
213	1.7354	3
420	1.5638	15
332	1.4584	15
204	1.4281	14
501	1.3853	3
224	1.3224	8
512	1.2566	11
440	1.2361	4
600, 404	1.1660	7
532	1.1199	8
424, 620	1.1060	12
116	1.0207	3
415, 613	1.0073	<2
444, 640	0.9701	5
316, 552	.9433	10
604	.9349	2
624	.9032	4
336, 732	.8814	5
800	.8743	<2
217	.8597	<2
820	.8480	2
516	.8304	5
644	.8245	4
536	.7872	5

Titanium Dioxide, brookite, TiO₂ (orthorhombic)

Powder data cards

Card number	Index lines	Source
3-0380	3. 47 2. 90 1. 88	British Museum.

Additional published patterns. Sturdivant and Pauling [1].

NBS sample. The sample of brookite was obtained from the U.S. National Museum. No. 97661 from Magnet Cove, Ark. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent silicon; 0.01 to 0.1 percent each of aluminum, iron, and vanadium; 0.001 to 0.01 percent magnesium.

The color of the sample was black. The indices of refraction were not determined because they were higher than 2.00.

The *d*-values of the three strongest lines are: 3.512, 2.900, and 3.465 Å.

Structural data. Sturdivant and Pauling [1] in 1928 determined that brookite has the space group D_{2h}¹⁵-Pcab (No. 61) and 8(TiO₂) per unit cell. Several lattice constants have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		<i>a</i>	<i>b</i>	<i>c</i>
		Å	Å	Å
1928	Sturdivant and Pauling [1].	5.447	9.185	5.145
1928	Schröder [2]-----	5.450	9.154	5.163
1932	Phillips [3]-----	5.44	9.20	5.14
1963	National Bureau of Standards at 25 °C.	^a 5.4558 ±.0004 ^b 5.456 ±.002	9.1819 ±.0007 9.174 ±.001	5.1429 ±.0003 5.138 ±.001

^a Sample described above.

^b Sample from the National Museum No. R2108 from von der Söule, Virven, Tyrol. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent iron; 0.01 to 0.1 percent each of magnesium, silicon, and vanadium; and 0.001 to 0.01 percent each of aluminum, barium, and manganese. The lattice constants given were derived from powder pattern data.

The density of brookite calculated from the NBS lattice constants (*a*) is 4.120 g/cm³ at 25 °C.

References

- [1] J. H. Sturdivant and L. Pauling, The crystal structure of brookite, *Z. Krist.* **68**, 239 (1928).
- [2] A. Schröder, Röntgenographische Feinbauuntersuchung am Brookit und über physikalische Eigenschaften der drei Titandioxyde, *Z. Krist.* **66**, 493 (1928).
- [3] F. C. Phillips, Crystals of brookite tabular parallel to the basal plane, *Min. Mag.* **23**, 126-129 (1932).

<i>hkl</i>	Internal Standard, Silver, <i>a</i> =4.0861 Å Cuλ=1.5405 Å at 25 °C	
	<i>d</i>	<i>I</i>
	Å	
120	3.512	100
111	3.465	79
121	2.900	91
200	2.729	4
012	2.476	23
201	2.409	18
131	2.370	6
220	2.344	4
211	2.332	4
040	2.296	5
112	2.254	8
022	2.244	18
221	2.133	16
032	1.9685	16
231	1.8934	28
132	1.8514	18
212	1.8332	3
240	1.7568	3
320	1.6908	21
241	1.6617	28
151	1.6486	5
113	1.6098	13
232	1.5968	2
123	1.5408	7
052	1.4942	10
160	1.4729	4
312	1.4656	9
251	1.4609	12
203	1.4515	12
152	1.4415	6
213	1.4336	10
161	1.4167	9
400	1.3640	5
332	1.3358	8
401	1.3186	3
233	1.3116	2
004	1.2852	2
024, 171	1.2381	10
431	1.2107	2
124	1.2074	1
333	1.1552	4
080	1.1480	2
441	1.1432	2
044	1.1217	4
521, 423	1.0399	3
281	1.0366	2
324	1.0237	4
125	0.9873	2
372, 254	.9829	4

Zinc Telluride, ZnTe (cubic)

Powder data cards

Card number	Index lines	Source
1-0582	3. 50 2. 14 1. 83	New Jersey Zinc Co.

Additional published patterns. None.

NBS sample. The sample of zinc telluride was obtained from Semi-Elements, Inc., Saxonburg, Pa. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent each of aluminum, barium, iron, and magnesium.

The color of the sample was reddish-brown. The indices of refraction were too high to be determined by the usual grain-immersion method.

The *d*-values of the three strongest lines are: 3.523, 2.159, and 1.840 Å.

Structural data. Zachariasen [1] in 1925 determined that zinc telluride has the zinc sulfide structure, the space group $T_d^2-F\bar{4}3m$ (No. 216), and 4[ZnTe] per unit cell. The unit cell measurement reported by Zachariasen has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		Å
1925	Zachariasen [1]-----	6. 101
1963	National Bureau of Standards at 25 °C-----	6. 1026

The density of zinc telluride calculated from the NBS lattice constant is 5.639 g/cm³ at 25 °C.

<i>hkl</i>	Internal Standard Tungsten, $a = 3.1648$ Å Cu, 1.5405 Å at 25 °C		
	<i>d</i>	<i>I</i>	<i>a</i>
	Å		Å
111	3. 523	100	6. 102
200	3. 051	10	6. 102
220	2. 159	81	6. 107
311	1. 840	37	6. 103
222	1. 762	3	6. 102
400	1. 526	8	6. 103
331	1. 4003	13	6. 104
420	1. 3645	3	6. 102
422	1. 2456	10	6. 102
511	1. 1745	7	6. 103
440	1. 0789	3	6. 1028
531	1. 0315	6	6. 1042
600	1. 0171	1	6. 1026
620	0. 9648	6	6. 1022
533	. 9307	3	6. 1028
622	. 9200	1	6. 1026
444	. 8808	1	6. 1026
711	. 8545	6	6. 1024
642	. 8155	8	6. 1026
731	. 7945	6	6. 1026
Average value of last five lines-----			6. 1026

Reference

- [1] W. Zachariasen, The crystal structure of the tellurides of zinc, cadmium, and mercury, Norsk. geol. Tidsskrift 8, 302-306 (1925).

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, AND 3⁵

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Aluminum orthophosphate, AlPO ₄ (orthorhombic)-----	10	4	Antimony telluride, Sb ₂ Te ₃ -----	3m	8
Aluminum oxide, (corundum), alpha Al ₂ O ₃ -----	9	3	Arsenic, As-----	3	6
Aluminum oxide monohydrate (böhmite), alpha Al ₂ O ₃ ·H ₂ O-----	3	38	Arsenic (III) iodide, AsI ₃ -----	6	17
Aluminum oxide monohydrate diaspore, beta Al ₂ O ₃ ·H ₂ O-----	3	41	Arsenic trioxide, claudetite, As ₂ O ₃ (monoclinic)-----	3m	9
Aluminum 3:2 silicate (mullite), 3Al ₂ O ₃ ·2SiO ₂ -----	3m	3	Arsenic trioxide (arsenolite), As ₂ O ₃ (cubic)-----	1	51
Ammonium aluminum sulfate dodecahydrate (teschermigite), NH ₄ Al(SO ₄) ₂ ·12H ₂ O-----	6	3	Barium, Ba-----	4	7
Ammonium azide, NH ₄ N ₃ -----	9	4	Barium arsenate, Ba ₃ (AsO ₄) ₂ -----	2m	6
Ammonium bicarbonate (teschemacherite), (NH ₄)HCO ₃ -----	9	5	Barium bromide monohydrate, BaBr ₂ ·H ₂ O-----	3m	10
Ammonium bromide, NH ₄ Br-----	2	49	Barium carbonate (witherite), BaCO ₃ (orthorhombic)-----	2	54
Ammonium bromosmate, (NH ₄)OsBr ₆ -----	3	71	Barium carbonate, BaCO ₃ (cubic) at 1075 °C-----	10	11
Ammonium bromoplatinate, (NH ₄) ₂ PtBr ₆ -----	9	6	Barium fluoride, BaF ₂ -----	1	70
Ammonium bromoselenate, (NH ₄) ₂ SeBr ₆ -----	8	4	Barium molybdate, BaMoO ₄ -----	7	7
Ammonium bromotellurate, (NH ₄) ₂ TeBr ₆ -----	8	5	Barium nitrate (nitrobarite), Ba(NO ₃) ₂ -----	1	81
Ammonium chloride (sal-ammoniac), NH ₄ Cl-----	1	59	Barium perchlorate trihydrate, Ba(ClO ₄) ₂ ·3H ₂ O-----	2m	7
Ammonium chloroiridate (NH ₄) ₂ IrCl ₆ -----	8	6	Barium peroxide, BaO ₂ -----	6	18
Ammonium chlorosmate, (NH ₄) ₂ OsCl ₆ -----	1m	6	Barium stannate, BaSnO ₃ -----	3m	11
Ammonium chloropalladate, (NH ₄) ₂ PdCl ₆ -----	8	7	Barium sulfate (barite), BaSO ₄ -----	3	65
Ammonium chloropalladite, (NH ₄) ₂ PdCl ₄ -----	6	6	Barium sulfide, BaS-----	7	8
Ammonium chloroplatinate, (NH ₄) ₂ PtCl ₆ -----	5	3	Barium titanate, BaTiO ₃ -----	3	45
Ammonium chlorostannate (NH ₄) ₂ SnCl ₆ -----	5	4	Barium tungstate, BaWO ₄ -----	7	9
Ammonium chlorotellurate, (NH ₄) ₂ TeCl ₆ -----	8	8	Barium zirconate, BaZrO ₃ -----	5	8
Ammonium chromium sulfate dodecahydrate, NH ₄ Cr(SO ₄) ₂ ·12H ₂ O-----	6	7	Beryllium aluminum oxide (chrysoberyl), BeAl ₂ O ₄ -----	9	10
Ammonium dihydrogen phosphate, NH ₄ H ₂ PO ₄ -----	4	64	Beryllium aluminum silicate, beryl, Be ₃ Al ₂ (SiO ₃) ₆ -----	9	13
Ammonium fluoberyllate, (NH ₄) ₂ BeF ₄ -----	3m	5	Beryllium chromium oxide, BeCr ₂ O ₄ -----	10	12
Ammonium fluoborate, NH ₄ BF ₄ -----	3m	6	Beryllium germanate, Be ₂ GeO ₄ -----	10	13
Ammonium fluogermanate, (NH ₄) ₂ GeF ₆ -----	6	8	Beryllium orthosilicate, phenacite, Be ₂ SiO ₄ -----	8	11
Ammonium fluosilicate (cryptohalite), (NH ₄) ₂ SiF ₆ -----	5	5	Beryllium oxide (bromellite), BeO-----	1	36
Ammonium gallium sulfate dodecahydrate, NH ₄ Ga(SO ₄) ₂ ·12H ₂ O-----	6	9	Bismuth, Bi-----	3	20
Ammonium iodide, NH ₄ I-----	4	56	Bismuth fluoride, BiF ₃ -----	1m	7
Ammonium iron sulfate dodecahydrate, NH ₄ Fe(SO ₄) ₂ ·12H ₂ O-----	6	10	Bismuth (III) iodide, BiI ₃ -----	6	20
Ammonium metavanadate, NH ₄ VO ₃ -----	8	9	Bismuth orthophosphate, BiPO ₄ (monoclinic)-----	3m	11
Ammonium nitrate (ammonia-niter), NH ₄ NO ₃ -----	7	4	Bismuth orthophosphate, BiPO ₄ (trigonal)-----	3m	13
Ammonium oxalate monohydrate (oxamite), (NH ₄) ₂ C ₂ O ₄ ·H ₂ O-----	7	5	Bismuth orthovanadate, low form, BiVO ₄ (tetragonal)-----	3m	14
Ammonium perchlorate, NH ₄ ClO ₄ , (orthorhombic)-----	7	6	Bismuth orthovanadate, high form, BiVO ₄ (monoclinic)-----	3m	14
Ammonium perrhenate, NH ₄ ReO ₄ -----	9	7	Bismuth oxybromide, BiOBr-----	8	14
Ammonium phosphomolybdate tetrahydrate, (NH ₄) ₃ PO ₄ (MoO ₃) ₁₂ ·4H ₂ O-----	8	10	Bismuth oxychloride (bismoclite), BiOCl-----	4	54
Ammonium sulfate (mascagnite), (NH ₄) ₂ SO ₄ (revised)-----	9	8	Bismuth oxyiodide, BiOI-----	9	16
Ammonium zirconium fluoride, (NH ₄) ₃ ZrF ₇ -----	6	14	Bismuth sulfide (bismuthinite), Bi ₂ S ₃ -----	4	23
Antimony, Sb-----	3	14	Bismuth telluride (tellurobismuthite), Bi ₂ Te ₃ -----	3m	16
Antimony (III) fluoride, SbF ₃ -----	2m	4	Bismuth trioxide (bismite), alpha Bi ₂ O ₃ -----	3m	17
			Cadmium, Cd-----	3	10
			Cadmium bromide, CdBr ₂ -----	9	17
			Cadmium carbonate (otavite), CdCO ₃ -----	7	11
			Cadmium chloride, CdCl ₂ -----	9	18
			Cadmium cyanide, Cd(CN) ₂ -----	2m	8
			Cadmium molybdate, CdMoO ₄ -----	6	21
			Cadmium oxide, CdO-----	2	27
			Cadmium perchlorate hexahydrate, Cd(ClO ₄) ₂ ·6H ₂ O-----	3m	19
			Cadmium selenide, CdSe, (hexagonal)-----	7	12
			Cadmium sulfate, CdSO ₄ -----	3m	20
			Cadmium sulfide (greenockite), CdS-----	4	15
			Cadmium telluride, CdTe-----	3m	21
			Cadmium tungstate, CdWO ₄ -----	2m	8

⁵ Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the accumulative index here is not necessarily the concluding index for the project.

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tri-Calcium aluminate, $3\text{CaO} \cdot \text{Al}_2\text{O}_3$ -----	5	10	Chromium orthophosphate, beta, CrPO_4 -----	9	26
Calcium aluminate 12:7, $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$ -----	9	20	Chromium (III) oxide, Cr_2O_3 -----	5	22
Calcium aluminum germanate, $\text{Ca}_3\text{Al}_2(\text{GeO}_4)_3$ -----	10	15	Chromium silicide, Cr_3Si -----	6	29
Calcium bromide hexahydrate, $\text{CaBr}_2 \cdot 6\text{H}_2\text{O}$ -----	8	15	Cobalt aluminum oxide, CoAl_2O_4 -----	9	27
Calcium carbonate (aragonite), CaCO_3 (or- thorhombic)-----	3	53	Cobalt arsenide (skutterudite), CoAs_3 -----	10	21
Calcium carbonate (calcite) CaCO_3 (hexag- onal)-----	2	51	Cobalt(II) carbonate (spherocobaltite), CoCO_3 -----	10	24
Calcium chromate, CaCrO_4 -----	7	13	Cobalt diarsenide, CoAs_2 -----	10	26
Calcium chromium germanate, $\text{Ca}_3\text{Cr}_2(\text{GeO}_4)_3$ -----	10	16	Cobaltfluosilicate hexahydrate, $\text{CoSiF}_6 \cdot 6\text{H}_2\text{O}$ -----	3m	27
Calcium chromium silicate (uvarovite), $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$ -----	10	17	Cobalt gallate, CoGa_2O_4 -----	10	27
Calcium fluoride (fluorite), CaF_2 -----	1	69	Cobalt germanate, Co_2GeO_4 -----	10	27
Calcium fluoride phosphate (fluorapatite), $\text{Ca}_5\text{F}(\text{PO}_4)_3$ -----	3m	22	Cobalt iron arsenide (safflorite), CoFeAs_4 -----	10	28
Calcium formate, $\text{Ca}(\text{HCO}_2)_2$ -----	8	16	Cobalt mercury thiocyanate, $\text{Co}[\text{Hg}(\text{CNS})_4]$ -----	2m	13
Calcium gallium germanate, $\text{Ca}_3\text{Ga}_2(\text{GeO}_4)_3$ -----	10	18	Cobalt(II) oxide, CoO -----	9	28
Calcium hydroxide (portlandite), $\text{Ca}(\text{OH})_2$ -----	1	58	Cobalt(II, III) oxide, Co_3O_4 -----	9	29
Calcium iron germanate, $\text{Ca}_3\text{Fe}_2(\text{GeO}_4)_3$ -----	10	19	Cobalt perchlorate hexahydrate, $\text{Co}(\text{ClO}_4)_2 \cdot$ $6\text{H}_2\text{O}$ -----	3m	28
Calcium iron silicate (andradite), $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ -----	9	22	Cobalt sulfate, beta, CoSO_4 -----	2m	14
Calcium molybdate (powellite), CaMoO_4 -----	6	22	Copper, Cu-----	1	15
Calcium nitrate, $\text{Ca}(\text{NO}_3)_2$ -----	7	14	Copper(I) bromide, CuBr -----	4	36
Calcium oxide, CaO -----	1	43	Copper carbonate basic, azurite, $\text{Cu}_3(\text{OH})_2$ $(\text{CO}_3)_2$ -----	10	30
Calcium sulfate (anhydrite), CaSO_4 -----	4	65	Copper carbonate, basic, (malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$ -----	10	31
Calcium sulfide (oldhamite), CaS -----	7	15	Copper(I) chloride (nantokite), CuCl -----	4	35
Calcium tungstate scheelite, CaWO_4 -----	6	23	Copper(I) iodide (marshite), CuI -----	4	38
Carbon, diamond, C-----	2	5	Copper(I) oxide (cuprite), Cu_2O -----	2	23
Cerium (III) chloride, CeCl_3 -----	1m	8	Copper(II) oxide (tenorite), CuO -----	1	49
Cerium (III) fluoride, CeF_3 -----	8	17	Copper sulfate (chalcocyanite), CuSO_4 -----	3m	29
Cerium, magnesium nitrate 24-hydrate, $\text{Ce}_2\text{Mg}_3(\text{NO}_3)_{12} \cdot 24\text{H}_2\text{O}$ -----	10	20	Copper(II) sulfide (covellite), CuS -----	4	13
Cerium niobium titanium oxide (eschynite), CeNbTiO_6 -----	3m	24	Dysprosium arsenate, DyAsO_4 -----	3m	30
Cerium (IV) oxide (cerianite) CeO_2 -----	1	56	Dysprosium gallium oxide 3:5, $\text{Dy}_3\text{Ga}_2(\text{GaO}_4)_3$ -----	2m	15
Cerium (III) vanadate, CeVO_4 -----	1m	9	Dysprosium sesquioxide, Dy_2O_3 -----	9	30
Cesium aluminum sulfate dodecahydrate, $\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	25	Erbium arsenate, ErAsO_4 -----	3m	31
Cesium bromate, CsBrO_3 -----	8	18	Erbium gallium oxide 3:5, $\text{Er}_3\text{Ga}_2(\text{GaO}_4)_3$ -----	1m	12
Cesium bromide, CsBr -----	3	49	Erbium manganite, ErMnO_3 -----	2m	16
Cesium bromoosmate (IV), Cs_2OsBr_6 -----	2m	10	Erbium phosphate, ErPO_4 -----	9	31
Cesium bromoplatinate, Cs_2PtBr_6 -----	8	19	Erbium sesquioxide, Er_2O_3 -----	8	25
Cesium bromoselenate, Cs_2SeBr_6 -----	8	20	Europium arsenate, EuAsO_4 -----	3m	32
Cesium bromotellurate, Cs_2TeBr_6 -----	9	24	Europium (III) chloride, EuCl_3 -----	1m	13
Cesium chlorate, CsClO_3 -----	8	20	Europium gallium oxide 3:5, $\text{Eu}_3\text{Ga}_2(\text{GaO}_4)_3$ -----	2m	17
Cesium chloride, CsCl -----	2	44	Europium oxychloride, EuOCl -----	1m	13
Cesium chloroosmate (IV), Cs_2OsCl_6 -----	2m	11	Gadolinium fluoride, GdF_3 -----	1m	14
Cesium chloroplatinate, Cs_2PtCl_6 -----	5	14	Gadolinium gallium oxide 3:5, $\text{Gd}_3\text{Ga}_2(\text{GaO}_4)_3$ -----	2m	18
Cesium chlorostannate, Cs_2SnCl_6 -----	5	16	Gadolinium oxide, Gd_2O_3 -----	1m	16
Cesium chromate, Cs_2CrO_4 -----	3m	25	Gadolinium oxychloride, GdOCl -----	1m	17
Cesium chromium sulfate dodecahydrate, $\text{CsCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	8	21	Gallium, Ga-----	2	9
Cesium dichloriodide, CsICl_2 -----	3	50	Gallium arsenide, GaAs -----	3m	33
Cesium fluoborate, CsBF_4 -----	8	22	Gallium antimonide, GaSb -----	6	30
Cesium fluogermanate, Cs_2GeF_6 -----	5	17	Gallium oxide, alpha, Ga_2O_3 -----	4	25
Cesium fluoplatinate, Cs_2PtF_6 -----	6	27	Gallium phosphate (α -quartz type), GaPO_4 -----	8	27
Cesium fluoride, CsF -----	3m	26	Germanium, Ge-----	1	18
Cesium fluosilicate, Cs_2SiF_6 -----	5	19	Germanium dioxide, GeO_2 (hexagonal) (low form)-----	1	51
Cesium gallium sulfate dodecahydrate, $\text{CsGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	8	23	Germanium dioxide, GeO_2 (tetragonal) (high form)-----	8	28
Cesium iodide, CsI -----	4	47	Germanium(IV) iodide, GeI_4 -----	5	25
Cesium iron sulfate dodecahydrate, $\text{CsFe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	28	Gold, Au-----	1	33
Cesium nitrate, CsNO_3 -----	9	25	Gold antimony 1:2 (aurostibite), AuSb_2 -----	7	18
Cesium perchlorate, CsClO_4 (orthorhombic)-----	1m	10	Gold(I) cyanide, AuCN -----	10	33
Cesium sulfate Cs_2SO_4 -----	7	17	Gold tin, 1:1 AuSn -----	7	19
Cesium vanadium sulfate dodecahydrate, $\text{CsV}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	1m	11	Hafnium, Hf-----	3	18
Chromium, Cr-----	5	20	Holmium arsenate, HoAsO_4 -----	3m	34
Chromium orthophosphate, alpha, CrPO_4 -----	2m	12	Holmium ethylsulfate nonahydrate, $\text{Ho}[(\text{C}_2\text{H}_5)_5\text{SO}_4]_3 \cdot 9\text{H}_2\text{O}$ -----	1m	18
m—Monograph 25.			Holmium sesquioxide, Ho_2O_3 -----	9	32
			Indium, In-----	3	12
			Indium antimony, InSb -----	4	73
			Indium arsenide, InAs -----	3m	35
			Indium oxide, In_2O_3 -----	5	26
			Indium phosphate, InPO_4 -----	8	29

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Iodic acid, HIO_3 -----	5	28	Magnesium germanate, Mg_2GeO_4 (cubic)---	10	37
Iodine, I_2 -----	3	16	Magnesium germanate, Mg_2GeO_4 (ortho- rhombic)-----	10	38
Iridium, Ir-----	4	9	Magnesium hydroxide (brucite), $\text{Mg}(\text{OH})_2$ ---	6	30
Iron, alpha Fe-----	4	3	Magnesium oxide (periclase), MgO -----	1	37
Iron arsenide, FeAs -----	1m	19	Magnesium silicate, enstatite, MgSiO_3 -----	6	32
Iron arsenide (loellingite), FeAs_2 -----	10	34	Magnesium silicate (forsterite), Mg_2SiO_4 -----	1	83
Iron sulfide (pyrite), FeS_2 -----	5	29	Magnesium silicate fluoride (norbergite), $\text{Mg}_2\text{SiO}_4\cdot\text{MgF}_2$ -----	10	39
Lanthanum arsenate, LaAsO_4 -----	3m	36	Magnesium silicate fluoride (humite), $3\text{Mg}_2\text{SiO}_4\cdot\text{MgF}_2$ -----	1m	30
Lanthanum borate, LaBO_3 -----	1m	20	Magnesium sulfate heptahydrate (epsomite), $\text{MgSO}_4\cdot 7\text{H}_2\text{O}$ -----	7	30
Lanthanum chloride, LaCl_3 -----	1m	21	Magnesium sulfide, MgS -----	7	31
Lanthanum fluoride, LaF_3 -----	7	21	Magnesium tin, Mg_2Sn -----	5	41
Lanthanum magnesium nitrate 24-hydrate, $\text{La}_2\text{Mg}_3(\text{NO}_3)_{12}\cdot 24\text{H}_2\text{O}$ -----	1m	22	Magnesium titanate (geikielite), MgTiO_3 ---	5	43
Lanthanum niobium titanium oxide, LaNbTiO_6 -----	3m	37	Magnesium tungstate, MgWO_4 -----	1	84
Lanthanum oxide, La_2O_3 -----	3	33	Manganese aluminate (galaxite), MnAl_2O_4 ---	9	35
Lanthanum oxychloride, LaOCl -----	7	22	Manganese(II) carbonate (rhodochrosite), MnCO_3 -----	7	32
Lead, Pb-----	1	34	Manganese ferrite (jacobsonite), MnFe_2O_4 ---	9	36
Lead bromide, PbBr_2 -----	2	47	Manganese(II) oxide (manganosite), MnO ---	5	45
Lead carbonate (cerussite), PbCO_3 -----	2	56	Manganese(III) oxide (partridgeite), Mn_2O_3 ---	9	37
Lead chloride (cotunnite), PbCl_2 -----	2	45	Manganese selenide, MnSe -----	10	41
Lead formate, $\text{Pb}(\text{HCO}_2)_2$ -----	8	30	Manganese sulfide (alabandite), alpha MnS -----	4	11
Lead fluochloride (matlockite), PbFCl ---	1	76	Manganese(II) tungstate (huebnerite), MnWO_4 -----	2m	24
Lead fluoride, alpha PbF_2 (orthorhombic)---	5	31	Mercury(I) bromide, Hg_2Br_2 -----	7	33
Lead fluoride, beta PbF_2 (cubic)-----	5	33	Mercury(I) chloride (calomel), Hg_2Cl_2 -----	1	72
Lead (II), iodide, PbI_2 -----	5	34	Mercury(II) chloride, HgCl_2 -----	1	73
Lead molybdate (wulfenite), PbMoO_4 -----	7	23	Mercury(II) cyanide, $\text{Hg}(\text{CN})_2$ -----	6	35
Lead monoxide (litharge), PbO (red) tetrag- onal-----	2	30	Mercury(II) fluoride, HgF_2 -----	2m	25
Lead monoxide (massicot), PbO (yellow) (orthorhombic)-----	2	32	Mercury(I) iodide, HgI_2 -----	4	49
Lead nitrate, $\text{Pb}(\text{NO}_3)_2$ -----	5	36	Mercury(II) iodide, HgI_2 -----	1	74
Lead (II, III) oxide (minium), Pb_3O_4 -----	8	32	Mercury(II) oxide (montroydite), HgO ---	9	39
Lead phosphate hydrate, $\text{Pb}_5(\text{PO}_4)_3\text{OH}$ -----	8	33	(revised)-----	7	35
Lead selenide (clausthalite), PbSe -----	5	38	Mercury(II) selenide (tiemannite), HgSe ---	7	35
Lead sulfate (anglesite), PbSO_4 -----	3	67	Mercury(II) sulfide (cinnabar), HgS (hex- agonal)-----	4	17
Lead sulfide (galena), PbS -----	2	18	Mercury(II) sulfide (metacinnabar), HgS (cubic)-----	4	21
Lead titanate, PbTiO_3 -----	5	39	Molybdenum, Mo-----	1	20
Lead tungstate (stolzite), PbWO_4 -----	7	24	Molybdenum disulfide (molybdenite), MoS_2 ---	5	47
Lithium arsenate, Li_3AsO_4 -----	2m	19	Molybdenum trioxide (molybdite), MoO_3 ---	3	30
Lithium bromide, LiBr -----	4	30	Neodymium borate, NdBO_3 -----	1m	32
Lithium chloride, LiCl -----	1	62	Neodymium chloride, NdCl_3 -----	1m	33
Lithium fluoride, LiF -----	1	61	Neodymium ethylsulfate nonahydrate, $\text{Nd}[(\text{C}_2\text{H}_5)_2\text{SO}_4]_3\cdot 9\text{H}_2\text{O}$ -----	9	41
Lithium iodate, LiIO_3 -----	7	26	Neodymium fluoride, NdF_3 -----	8	36
Lithium molybdate, Li_2MoO_4 , (trigonal)-----	1m	23	Neodymium gallium oxide 3:5, $\text{Nd}_3\text{Ga}_2(\text{GaO}_4)_3$ -----	1m	34
Lithium oxide, Li_2O -----	1m	25	Neodymium oxide, Nd_2O_3 -----	4	26
Lithium nitrate, LiNO_3 -----	7	27	Neodymium oxychloride, NdOCl -----	8	37
Lithium perchlorate trihydrate, $\text{LiClO}_4\cdot 3\text{H}_2\text{O}$ ---	8	34	Nickel, Ni-----	1	13
Lithium phosphate, low form, (lithiophos- phate), Li_3PO_4 -----	3m	38	Nickel aluminate, NiAl_2O_4 -----	9	42
Lithium phosphate, high form, Li_3PO_4 -----	3m	39	Nickel arsenic 1:2 (rammelsbergite), NiAs_2 ---	10	42
Lithium trimetaphosphate trihydrate, $\text{Li}_3\text{P}_3\text{O}_9\cdot 3\text{H}_2\text{O}$ -----	2m	20	Nickel arsenic sulfide (gersdorffite), NiAsS ---	1m	35
Lithium tungstate, Li_2WO_4 , (trigonal)-----	1m	25	Nickel (II) carbonate, NiCO_3 (trigonal)---	1m	36
Lithium tungstate hemihydrate, $\text{Li}_2\text{WO}_4\cdot \frac{1}{2}\text{H}_2\text{O}$ -----	2m	20	Nickel ferrite (trevorite), NiFe_2O_4 -----	10	44
Lutetium gallium oxide 3:5, $\text{Lu}_3\text{Ga}_2(\text{GaO}_4)_3$ ---	2m	22	Nickel fluosilicate hexahydrate, $\text{NiSiF}_6\cdot 6\text{H}_2\text{O}$ ---	8	38
Lutetium manganite, LuMnO_3 -----	2m	23	Nickel gallate, NiGa_2O_4 -----	10	45
Lutetium oxide, Lu_2O_3 -----	1m	27	Nickel germanate, Ni_2GeO_4 -----	9	43
Magnesium, Mg-----	1	10	Nickel (II) oxide (bunsenite), NiO -----	1	47
Magnesium aluminate (spinel), MgAl_2O_4 ---	2	35	Nickel sulfate, NiSO_4 -----	2m	26
Magnesium aluminum silicate (low-cordi- erite), $\text{Mg}_2\text{Al}_3\text{Si}_5\text{O}_{18}$ (orthorhombic)---	1m	28	Nickel sulfate hexahydrate (retgersite), $\text{NiSO}_4\cdot 6\text{H}_2\text{O}$ -----	7	36
Magnesium aluminum silicate (high-cordi- erite), $\text{Mg}_2\text{Al}_3\text{Si}_5\text{O}_{18}$ (hexagonal)---	1m	29	Nickel sulfide, millerite, NiS -----	1m	37
Magnesium ammonium phosphate hexahy- drate, (struvite), $\text{MgNH}_4\text{PO}_4\cdot 6\text{H}_2\text{O}$ -----	3m	41	Nickel tungstate, NiWO_4 -----	2m	27
Magnesium carbonate (magnesite), MgCO_3 ---	7	28	Niobium silicide, NbSi_2 -----	8	39
Magnesium chromite (picrochromite), MgCr_2O_4 -----	9	34	Osmium, Os-----	4	8
Magnesium fluoride (sellaite), MgF_2 -----	4	33	Palladium, Pd-----	1	21
Magnesium gallate, MgGa_2O_4 -----	10	36	Palladium oxide, PdO -----	4	27

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Potassium aluminum sulfate dodecahydrate (alum), $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	36	Samarium fluoride, SmF_3 -----	1m	41
Potassium borohydride, KBH_4 -----	9	44	Samarium gallium oxide 3:5, $\text{Sm}_3\text{Ga}_2(\text{GaO}_4)_3$ -----	1m	42
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Potassium bromide, KBr -----	1	66	Scandium oxide, Sc_2O_3 -----	3	27
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Potassium bromoselenate, K_2SeBr_6 -----	8	41	Selenium, Se-----	5	54
Potassium chlorate, KClO_3 -----	3m	42	Selenium dioxide (selenolite), SeO_2 -----	1	53
Potassium chloride (sylvite), KCl -----	1	65	Silicon, Si-----	2	6
Potassium chloroplatinate, K_2PtCl_6 -----	5	49	Silicon dioxide alpha or low quartz, SiO_2 (hexagonal)-----	3	24
Potassium chlororhenate, K_2ReCl_6 -----	2m	28	Silicon dioxide (alpha or low cristobalite), SiO_2 (Revised) (tetragonal)-----	10	48
Potassium chlororuthenate (IV), K_2RuCl_6 -----	10	46	Silicon dioxide (beta or high cristobalite), SiO_2 (cubic)-----	1	42
Potassium chlorostannate, K_2SnCl_6 -----	6	38	Silver, Ag-----	1	23
Potassium chromium sulfate dodecahydrate, $\text{KCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	39	Silver antimony telluride, AgSbTe_2 -----	3m	47
Potassium cobaltinitrite, $\text{K}_3\text{Co}(\text{NO}_2)_6$ -----	9	45	Silver arsenate, Ag_3AsO_4 -----	5	56
Potassium cyanate, KCNO -----	7	39	Silver bromate, AgBrO_3 -----	5	57
Potassium cyanide, KCN -----	1	77	Silver bromide (bromyrite), AgBr -----	4	46
Potassium dihydrogen arsenate, KH_2AsO_4 -----	1m	38	Silver carbonate, Ag_2CO_3 -----	1m	44
Potassium dihydrogen phosphate, KH_2PO_4 -----	3	69	Silver chlorate, AgClO_3 -----	7	44
Potassium fluogermanate, K_2GeF_6 -----	6	41	Silver chloride, (cerargyrite), AgCl -----	4	44
Potassium fluoplatinate, K_2PtF_6 -----	6	42	Silver iodide (iodyrite), AgI (hexagonal)-----	8	51
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Potassium fluosilicate (hieratite), K_2SiF_6 -----	5	50	Silver metaperiodate, AgIO_4 -----	9	49
Potassium fluotitanate, K_2TiF_6 -----	7	40	Silver molybdate, Ag_2MoO_4 -----	7	45
Potassium heptafluozirconate, K_3ZrF_7 -----	9	46	Silver nitrate, AgNO_3 -----	5	59
Potassium hydroxy-chlororuthenate, $\text{K}_4\text{Ru}_2\text{Cl}_{10}\text{O} \cdot \text{H}_2\text{O}$ -----	10	47	Silver nitrite, AgNO_2 -----	5	60
Potassium iodide, KI -----	1	68	Silver oxide, Ag_2O -----	1m	45
Potassium lithium sulfate, KLiSO_4 -----	3m	43	Silver (II) oxynitrate, $\text{Ag}_7\text{O}_8\text{NO}_3$ -----	4	61
Potassium metaperiodate, KIO_4 -----	7	41	Silver perhenate, AgReO_4 -----	8	53
Potassium nitrate (niter), KNO_3 -----	3	58	Silver phosphate, Ag_3PO_4 -----	5	62
Potassium nitroso chlororuthenate, $\text{K}_2\text{RuCl}_6\text{NO}$ -----	2m	29	Silver selenate, Ag_2SeO_4 -----	2m	32
Potassium perchlorate, KClO_4 -----	6	43	Silver sulfate, Ag_2SO_4 -----	7	46
Potassium perchromate, K_3CrO_8 -----	3m	44	Silver sulfide (argentite), Ag_2S -----	10	51
Potassium permanganate, KMnO_4 -----	7	42	Sodium acid fluoride, NaHF_2 -----	5	63
Potassium perhenate, KReO_4 -----	8	41	Sodium borohydride, NaBH_4 -----	9	51
Potassium phosphomolybdate, tetrahydrate, $\text{K}_2\text{PO}_4(\text{MoO}_3)_{12} \cdot 4\text{H}_2\text{O}$ -----	8	43	Sodium bromate, NaBrO_3 -----	5	65
Potassium sulfate (arcanite), K_2SO_4 -----	3	62	Sodium bromide, NaBr -----	3	47
Potassium thiocyanate, KCNS -----	8	44	Sodium carbonate monohydrate (thermona- trite), $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ -----	8	54
Potassium zinc decavanadate 16 hydrate, $\text{K}_2\text{Zn}_2\text{V}_{10}\text{O}_{28} \cdot 16\text{H}_2\text{O}$ -----	3m	45	Sodium chlorate, NaClO_3 -----	3	51
Potassium zinc fluoride, KZnF_3 -----	5	51	Sodium chloride (halite), NaCl -----	2	41
Praseodymium chloride, PrCl_3 -----	1m	39	Sodium cyanate, NaCNO -----	2m	33
Praseodymium fluoride, PrF_3 -----	5	52	Sodium cyanide, NaCN (cubic)-----	1	78
Praseodymium oxychloride, PrOCl -----	9	47	Sodium cyanide, NaCN (orthorhombic) at 6 °C-----	1	79
Rhenium, Re-----	2	13	Sodium fluoride (villiaumite), NaF -----	1	63
Rhodium, Rh-----	3	9	Sodium iodate, NaIO_3 -----	7	47
Rubidium aluminum sulfate dodecahydrate, $\text{RbAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	44	Sodium iodide, NaI -----	4	31
Rubidium bromate, RbBrO_3 -----	8	45	Sodium magnesium aluminum boron hy- droxy silicate, dravite, $\text{NaMg}_3\text{Al}_6\text{B}_3\text{Si}_6\text{O}_{27}(\text{OH})_4$ -----	3m	47
Rubidium bromide, RbBr -----	7	43	Sodium metaperiodate, NaIO_4 -----	7	48
Rubidium bromotellurate, Rb_2TeBr_6 -----	8	46	Sodium molybdate, Na_2MoO_4 -----	1m	46
Rubidium chlorate, RbClO_3 -----	8	47	Sodium nitrate (soda-niter), NaNO_3 -----	6	50
Rubidium chloride, RbCl -----	4	41	Sodium nitrite, NaNO_2 -----	4	62
Rubidium chloroplatinate, Rb_2PtCl_6 -----	5	53	Sodium orthotungstate (VI) dihydrate, $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$ -----	2m	33
Rubidium chlorostannate, Rb_2SnCl_6 -----	6	46	Sodium perchlorate, NaClO_4 (orthorhombic)-----	7	49
Rubidium chlorotellurate, Rb_2TeCl_6 -----	8	48	Sodium sulfate (thenardite), Na_2SO_4 -----	2	59
Rubidium chromate, Rb_2CrO_4 -----	3m	46	Sodium sulfite, Na_2SO_3 -----	3	60
Rubidium chromium sulfate dodecahydrate, $\text{RbCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	47	Sodium tetrametaphosphate tetrahydrate, alpha, $\text{Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (monoclinic)-----	10	52
Rubidium fluoplatinate, Rb_2PtF_6 -----	6	48	Sodium tetrametaphosphate tetrahydrate, beta, $\text{Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (triclinic)-----	2m	35
Rubidium fluosilicate, Rb_2SiF_6 -----	6	49	Sodium trimetaphosphate, $\text{Na}_3\text{P}_3\text{O}_9$ -----	3m	49
Rubidium iodide, RbI -----	4	43	Sodium trimetaphosphate monohydrate, $\text{Na}_3\text{P}_3\text{O}_9 \cdot \text{H}_2\text{O}$ -----	3m	50
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Rubidium periodate, RbIO_4 -----	2m	31	Stannous fluoride, SnF_2 -----	3m	51
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Strontium chloride, SrCl_2 -----	4	40	Thulium sesquioxide, Tm_2O_3 -----	9	58
Strontium chloride hexahydrate, $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ -----	4	58	Tin, alpha, Sn (cubic)-----	2	12
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Strontium formate, $\text{Sr}(\text{CHO}_2)_2$ -----	8	55	Tin(IV) iodide, SnI_4 -----	5	71
Strontium formate dihydrate, $\text{Sr}(\text{CHO}_2)_2 \cdot 2\text{H}_2\text{O}$ (orthorhombic)-----	8	56	Tin(II) oxide, SnO -----	4	28
Strontium iodide hexahydrate, $\text{SrI}_2 \cdot 6\text{H}_2\text{O}$ -----	8	58	Tin (IV) oxide (cassiterite), SnO_2 -----	1	54
Strontium molybdate, SrMoO_4 -----	7	50	Tin(II) telluride, SnTe -----	7	61
Strontium nitrate, $\text{Sr}(\text{NO}_3)_2$ -----	1	80	Titanium, Ti-----	3	1
Strontium oxide, SrO -----	5	68	Titanium dioxide (anatase), TiO_2 (tetra- gonal)-----	1	46
Strontium peroxide, SrO_2 -----	6	52	Titanium dioxide, brookite, TiO_2 (ortho- rhombic)-----	3m	57
Strontium sulfate (celestite), SrSO_4 -----	2	61	Titanium dioxide (rutile), TiO_2 (tetragonal)-----	1	44
Strontium sulfide, SrS -----	7	52	Titanium(III) oxide, $\text{TiO}_{1.515}$ -----	9	59
Strontium titanate, SrTiO_3 -----	3	44	Titanium silicide, Ti_5Si_3 -----	8	64
Strontium tungstate, SrWO_4 -----	7	53	Tungsten, W-----	1	28
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Thallium(I) chlorate, TlClO_3 -----	8	61	Zinc cyanide, $\text{Zn}(\text{CN})_2$ -----	5	73
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Thallium chloroplatinate, Tl_2PtCl_6 -----	5	70	Zinc fluosilicate hexahydrate, $\text{ZnSiF}_6 \cdot 6\text{H}_2\text{O}$ -----	8	70
Thallium chlorostannate, Tl_2SnCl_6 -----	6	54	Zinc germanate, Zn_2GeO_4 -----	10	56
Thallium chromate, Tl_2CrO_4 -----	3m	54	Zinc iodide, ZnI_2 -----	9	60
Thallium chromium sulfate dodecahydrate, $\text{TlCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	55	Zinc orthosilicate (willemite), Zn_2SiO_4 -----	7	62
Thallium fluosilicate, Tl_2SiF_6 -----	6	56	Zinc oxide (zincite), ZnO -----	2	25
Thallium gallium sulfate dodecahydrate, $\text{TlGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ -----	6	57	Zinc pyrosilicate hydrate, hemimorphite, $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$ -----	2	62
Thallium(I) iodate, TlIO_3 -----	8	62	Zinc selenide, ZnSe -----	3	23
Thallium(I) iodide, TII (orthorhombic)-----	4	53	Zinc sulfate (zinkosite), ZnSO_4 -----	7	64
Thallium(I) nitrate, TlNO_3 -----	6	58	Zinc sulfate heptahydrate (goslarite), $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ -----	8	71
Thallium(III) oxide, Tl_2O_3 -----	2	28	Zinc sulfide, (wurtzite), alpha ZnS (hexag- onal)-----	2	14
Thallium(I) perchlorate, TlClO_4 -----	2m	38	Zinc sulfide, (sphalerite), beta ZnS (cubic)-----	2	16
Thallium(I) phosphate, Tl_3PO_4 -----	7	58	Zinc telluride, ZnTe -----	3m	58
Thallium(III) phosphate, TlPO_4 -----	7	59	Zinc tungstate, (sanmartinite), ZnWO_4 -----	2m	40
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			Zirconium silicate zircon, ZrSiO_4 -----	4	68
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*Beryl, $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ -----	9	13	Molybdenite, MoS_2 -----	5	47
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*Brookite, TiO_2 -----	3m	57	Norbergite, $\text{Mg}_2\text{SiO}_4 \cdot \text{MgF}_2$ -----	10	39
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Celestite, SrSO_4 -----	2	61	Partridgeite, Mn_2O_3 -----	9	37
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Cristobalite, (alpha or low) SiO_2 (revised)-----	10	48	Selenolite, SeO_2 -----	1	53
Cristobalite, (beta or high) SiO_2 -----	1	42	Sellaite, MgF_2 -----	4	33
Cryptohalite, $(\text{NH}_4)_2\text{SiF}_6$ -----	5	5	Senarmontite, Sb_2O_3 -----	3	31
Cuprite, Cu_2O -----	2	23	Skutterudite, CoAs_3 -----	10	21
*Diamond, C -----	2	5	*Smithsonite, ZnCO_3 -----	8	69
*Diaspore, $\text{Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ -----	3	41	Soda-niter, NaNO_3 -----	6	50
*Dravite, $\text{NaMg}_3\text{Al}_6\text{B}_3\text{Si}_6\text{O}_{27}(\text{OH})_4$ -----	3m	47	Sphalerite, ZnS -----	2	16
*Enstatite, MgSiO_3 -----	6	32	Spherochalcite, CoCO_3 -----	10	24
Epsomite, $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ -----	7	30	Spinel, MgAl_2O_4 -----	2	35
Eschynite, CeNbTiO_6 -----	3m	24	Stibnite, Sb_2S_3 -----	5	6
Ettringite, $\text{Al}_2\text{O}_3 \cdot 6\text{CaO} \cdot 3\text{SO}_3 \cdot 31\text{H}_2\text{O}$ -----	8	3	Stolzite, PbWO_4 -----	7	24
Fluoroapatite, $\text{Ca}_5\text{F}(\text{PO}_4)_3$ -----	3m	22	Strontianite, SrCO_3 -----	3	56
Fluorite, CaF_2 -----	1	69	Struvite, $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ -----	3m	41
Forsterite, Mg_2SiO_4 -----	1	83	Sylvite, KCl -----	1	65
Galaxite, MnAl_2O_4 -----	9	35	*Tellurite, TeO_2 -----	9	57
Galena, PbS -----	2	18	Tellurobismuthite, Bi_2Te_3 -----	3m	16
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*Hemimorphite, $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$ -----	2	62	Tiemannite, HgSe -----	7	35
Hieratite, K_2SiF_6 -----	5	50	*Topaz, $\text{Al}_2\text{SiO}_4(\text{F}, \text{OH})_2$ -----	1m	4
Huebnerite, MnWO_4 -----	2m	24	Trevorite, NiFe_2O_4 -----	10	44
Humite, $3\text{Mg}_2\text{SiO}_4 \cdot \text{MgF}_2$ -----	1m	30	Tungstenite, WS_2 -----	8	65
Iodyrite, AgI -----	8	51	Uraninite, UO_2 -----	2	33
Jacobsite, MnFe_2O_4 -----	9	36	Uvarovite, $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$ -----	10	17
Litharge, PbO (red)-----	2	30	*Valentinite, Sb_2O_3 -----	10	6
Lithiophosphate, Li_3PO_4 -----	3m	38	Villiaumite, NaF -----	1	63
Loellingite, FeAs_2 -----	10	34	Willemite, Zn_2SiO_4 -----	7	62
Magnesite, MgCO_3 -----	7	28	Witherite, BaCO_3 -----	2	54
Malachite, $\text{Cu}_2(\text{OH})_2\text{CO}_3$ -----	10	31	Wulfenite, PbMoO_4 -----	7	23
Manganosite, MnO -----	5	45	Wurtzite, ZnS -----	2	14
Marshite, CuI -----	4	38	Xenotime, YPO_4 -----	8	67
Mascagnite, $(\text{NH}_4)_2\text{SO}_4$ (revised)-----	9	8	Zincite, ZnO -----	2	25
			Zinkosite, ZnSO_4 -----	7	64
			*Zircon, ZrSiO_4 -----	4	68

*Natural mineral.
m—Monograph 25.

